

PMID- 26755143
OWN - NLM
STAT- In-Data-Review
DA - 20160112
IS - 1873-4324 (Electronic)
IS - 0003-2670 (Linking)
VI - 905
DP - 2016 Jan 28
TI - Ultraviolet irradiation-induced substitution of fluorine with hydroxyl radical for mass spectrometric analysis of perfluorooctane sulfonyl fluoride.
PG - 100-5
LID - 10.1016/j.aca.2015.11.044 [doi]
LID - S0003-2670(15)30037-4 [pii]
AB - A rapid and solvent free substitution reaction of a fluorine atom in perfluorooctane sulfonyl fluoride (PFOSF) with a hydroxyl radical is reported. Under irradiation of ultraviolet laser on semiconductor nanoparticles or metal surfaces, hydroxyl radicals can be generated through hole oxidization. Among all fluorine atoms of PFOSF, highly active hydroxyl radicals specifically substitute the fluorine of sulfonyl fluoride functional group. Resultant perfluorooctane sulfonic acid is further ionized through capture of photo-generated electrons that switch the neutral molecules to negatively charged odd electron hypervalent ions. The unpaired electron subsequently initiates alpha O-H bond cleavage and produces perfluorooctane sulfonate negative ions. Hydroxyl radical substitution and molecular dissociation of PFOSF have been confirmed by masses with high accuracy and resolution. It has been applied to direct mass spectrometric imaging of PFOSF adsorbed on surfaces of plant leaves.
CI - Copyright (c) 2015 Elsevier B.V. All rights reserved.
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LA - eng

PT - Journal Article

DEP - 20151217

PL - Netherlands

TA - Anal Chim Acta

JT - Analytica chimica acta

JID - 0370534

SB - IM

OTO - NOTNLM

OT - Hydroxyl radical

OT - Imaging mass spectrometry

OT - Perfluorooctane sulfonyl fluoride

OT - Plant chemicals

OT - Substitution

EDAT- 2016/01/13 06:00

MHDA- 2016/01/13 06:00

CRDT- 2016/01/13 06:00

PHST- 2015/09/10 [received]

PHST- 2015/11/21 [revised]

PHST- 2015/11/26 [accepted]

PHST- 2015/12/17 [aheadofprint]

AID - S0003-2670(15)30037-4 [pii]

AID - 10.1016/j.aca.2015.11.044 [doi]

PST - ppublish

SO - Anal Chim Acta. 2016 Jan 28;905:100-5. doi: 10.1016/j.aca.2015.11.044. Epub 2015 Dec 17.

PMID- 26714691

OWN - NLM

STAT- Publisher

DA - 20151230

LR - 20151231

IS - 1432-0703 (Electronic)

IS - 0090-4341 (Linking)

DP - 2015 Dec 29

TI - Perfluoroalkyl Acid Concentrations in Livers of Fox (*Vulpes vulpes*) and Chamois (*Rupicapra rupicapra*) from Germany and Austria.

AB - The concentrations of 11 perfluorinated alkyl acids (PFAAs) were measured in the

livers of foxes (*Vulpes vulpes*) from Germany, a primarily carnivorous species, and chamois (*Rupicapra rupicapra*) from Austria, an herbivorous species. Perfluorooctanesulfonate (PFOS) at concentrations [all results refer to wet weight (ww)] of 3.2-320 microg/kg were detected in all 40 fox livers tested, yielding an arithmetic mean of 46.6 microg/kg and a median of 29.8 microg/kg. Long-chain PFAAs were detected at concentrations of 1.7 microg/kg perfluorononanoic acid (PFNA) to 2.4 microg/kg perfluorodecanoic acid (PFDA) and perfluorododecanoic acid (PFDoDA). Of the short-chain PFAAs tested, only perfluorohexanoic acid (PFHxA) was found in 1 fox liver at a concentration of 1.4 microg/kg, and perfluorohexane sulfonate (PFHxS) was found in 2 fox livers at a concentration of 1 microg/kg each. PFOS and PFNA concentrations higher than limit of quantification (LOQ) were detected in 90.9 and 81.8 % of chamois livers, respectively. The arithmetic mean for PFOS concentrations was 2.2 microg/kg (median 2.4 microg/kg), a factor of 21 (median factor of 12) lower than in fox livers. The arithmetic mean for PFNA concentrations was 2.0 microg/kg (median 1.9 microg/kg). Perfluorobutanoic acid, PFHxA, perfluorooctanoic acid, perfluorobutanesulfonate, and PFHxS were not detected at concentrations higher than the LOQ in any of the samples. The various results are compared with one another and with the results of other studies of herbivorous, carnivorous, and omnivorous wild animals. The highest concentrations of PFAA, in particular PFOS, were found in omnivorous animals followed by carnivores. The lowest levels were present in herbivores.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151229

TA - Arch Environ Contam Toxicol

JT - Archives of environmental contamination and toxicology

JID - 0357245

EDAT- 2015/12/31 06:00
 MHDA- 2015/12/31 06:00
 CRDT- 2015/12/31 06:00
 PHST- 2015/09/25 [received]
 PHST- 2015/11/30 [accepted]
 PHST- 2015/12/29 [aheadofprint]
 AID - 10.1007/s00244-015-0250-8 [doi]
 AID - 10.1007/s00244-015-0250-8 [pii]
 PST - aheadofprint
 SO - Arch Environ Contam Toxicol. 2015 Dec 29.

PMID- 26734112
 OWN - NLM
 STAT- PubMed-not-MEDLINE
 DA - 20160106
 DCOM- 20160106
 LR - 20160108
 IS - 1860-5397 (Electronic)
 VI - 11
 DP - 2015
 TI - Carbon-carbon bond cleavage for Cu-mediated aromatic trifluoromethylations and pentafluoroethylations.
 PG - 2661-70
 LID - 10.3762/bjoc.11.286 [doi]
 AB - This short review highlights the copper-mediated fluoroalkylation using perfluoroalkylated carboxylic acid derivatives. Carbon-carbon bond cleavage of perfluoroalkylated carboxylic acid derivatives takes place in fluoroalkylation reactions at high temperature (150-200 degrees C) or under basic conditions to generate fluoroalkyl anion sources for the formation of fluoroalkylcopper species. The fluoroalkylation reactions, which proceed through decarboxylation or tetrahedral intermediates, are useful protocols for the synthesis of fluoroalkylated aromatics.

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LA - eng
PT - Journal Article
PT - Review
DEP - 20151218
PL - Germany
TA - Beilstein J Org Chem
JT - Beilstein journal of organic chemistry
JID - 101250746
PMC - PMC4685791
OID - NLM: PMC4685791
OTO - NOTNLM
OT - carbon-carbon bond cleavage
OT - decarboxylation
OT - fluoral
OT - tetrahedral intermediate
OT - trifluoroacetate
OT - trifluoromethylation
OT - beta-carbon elimination
EDAT- 2016/01/07 06:00
MHDA- 2016/01/07 06:01
CRDT- 2016/01/07 06:00
PHST- 2015 [ecollection]
PHST- 2015/09/30 [received]
PHST- 2015/12/11 [accepted]
PHST- 2015/12/18 [epublish]
AID - 10.3762/bjoc.11.286 [doi]
PST - epublish
SO - Beilstein J Org Chem. 2015 Dec 18;11:2661-70. doi: 10.3762/bjoc.11.286.
eCollection 2015.

PMID- 26713315
OWN - NLM
STAT- In-Data-Review
DA - 20151229
LR - 20151231
IS - 2314-6141 (Electronic)
VI - 2015
DP - 2015
TI - Overview of Emerging Contaminants and Associated Human Health Effects.
PG - 404796
LID - 10.1155/2015/404796 [doi]
AB - In recent decades, because of significant progress in the analysis and detection of trace pollutants, emerging contaminants have been discovered and quantified in living beings and diverse environmental substances; however, the adverse effects of environmental exposure on the general population are largely unknown. This review summarizes the conclusions of the comprehensive epidemic literature and representative case reports relevant to emerging contaminants and the human body to address concerns about potential harmful health effects in the general

population. The most prevalent emerging contaminants include perfluorinated compounds, water disinfection byproducts, gasoline additives, manufactured nanomaterials, human and veterinary pharmaceuticals, and UV-filters. Rare but statistically meaningful connections have been reported for a number of contaminants and cancer and reproductive risks. Because of contradictions in the outcomes of some investigations and the limited number of articles, no significant conclusions regarding the relationship between adverse effects on humans and extents of exposure can be drawn at this time. Here, we report that the current evidence is not conclusive and comprehensive and suggest prospective cohort studies in the future to evaluate the associations between human health outcomes and emerging environmental contaminants.

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LA - eng

PT - Journal Article

PT - Review

DEP - 20151202

PL - United States

TA - Biomed Res Int

JT - BioMed research international

JID - 101600173

SB - IM

PMC - PMC4680045
OID - NLM: PMC4680045
EDAT- 2015/12/30 06:00
MHDA- 2015/12/30 06:00
CRDT- 2015/12/30 06:00
PHST- 2015/09/11 [received]
PHST- 2015/11/16 [revised]
PHST- 2015/11/17 [accepted]
PHST- 2015/12/02 [epublish]
AID - 10.1155/2015/404796 [doi]
PST - ppublish
SO - Biomed Res Int. 2015;2015:404796. doi: 10.1155/2015/404796. Epub 2015 Dec 2.

PMID- 26451660
OWN - NLM
STAT- In-Data-Review
DA - 20151120
IS - 1364-548X (Electronic)
IS - 1359-7345 (Linking)
VI - 51
IP - 96
DP - 2015 Dec 14
TI - TfOH-catalyzed domino cycloisomerization/hydrolytic defluorination of 2,3-allenyl perfluoroalkyl ketones.
PG - 17112-5
LID - 10.1039/c5cc06111c [doi]
AB - A unique TfOH-catalyzed domino cycloisomerization/hydrolytic defluorination reaction of easily available n-perfluoroalkyl allenones in the presence of H₂O providing furanyl perfluoroalkyl ketones has been developed. The (18)O-labelling experiments confirmed that the oxygen atom of the carbonyl group in the final products originates from water.
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LA - eng

PT - Journal Article

PL - England

TA - Chem Commun (Camb)

JT - Chemical communications (Cambridge, England)

JID - 9610838

SB - IM

EDAT- 2015/10/10 06:00

MHDA- 2015/10/10 06:00

CRDT- 2015/10/10 06:00

PHST- 2015/10/09 [aheadofprint]

PHST- 2015/11/19 [epublish]

AID - 10.1039/c5cc06111c [doi]

PST - ppublish

SO - Chem Commun (Camb). 2015 Dec 14;51(96):17112-5. doi: 10.1039/c5cc06111c.

PMID- 26496824

OWN - NLM

STAT- In-Data-Review

DA - 20160115

IS - 1521-3765 (Electronic)

IS - 0947-6539 (Linking)

VI - 21

IP - 52

DP - 2015 Dec 21

TI - Enantioselective NHC-Catalyzed Redox [2+2] Cycloadditions with Perfluoroketones:
A Route to Fluorinated Oxetanes.

PG - 18944-8

LID - 10.1002/chem.201504256 [doi]

AB - The N-heterocyclic carbene (NHC) catalyzed redox formal [2+2] cycloaddition

between alpha-aryloxyaldehydes and perfluoroketones, followed by ring-opening in situ delivers a variety of perfluorinated beta-hydroxycarbonyl compounds in good yield, and excellent diastereo- and enantioselectivity. Through a reductive work-up and subsequent cyclization, this protocol offers access to highly substituted fluorinated oxetanes in two steps and in high ee.

CI - (c) 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

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LA - eng

PT - Journal Article

DEP - 20151123

PL - Germany

TA - Chemistry

JT - Chemistry (Weinheim an der Bergstrasse, Germany)

JID - 9513783

SB - IM

OTO - NOTNLM

OT - Lewis base

OT - N-heterocyclic carbene

OT - organocatalysis

OT - oxetane

OT - pentafluoroethyl

EDAT- 2015/10/27 06:00

MHDA- 2015/10/27 06:00

CRDT- 2015/10/27 06:00

PHST- 2015/10/22 [received]

PHST- 2015/11/23 [aheadofprint]

AID - 10.1002/chem.201504256 [doi]

PST - ppublish

SO - Chemistry. 2015 Dec 21;21(52):18944-8. doi: 10.1002/chem.201504256. Epub 2015 Nov 23.

PMID- 26624955

OWN - NLM

STAT- In-Data-Review

DA - 20151228

IS - 1879-1298 (Electronic)

IS - 0045-6535 (Linking)
VI - 144
DP - 2016 Feb
TI - Aerobic biodegradation of toluene-2,4-di(8:2 fluorotelomer urethane) and hexamethylene-1,6-di(8:2 fluorotelomer urethane) monomers in soils.
PG - 2482-8
LID - 10.1016/j.chemosphere.2015.11.021 [doi]
LID - S0045-6535(15)30354-4 [pii]
AB - Aerobic soil biodegradation of toluene-2,4-di(8:2 fluorotelomer urethane) (FTU) and hexamethylene-1,6-di(8:2 fluorotelomer urethane) (HMU) in a forest soil and FTU in an agricultural silty clay loam soil was monitored for up to 6 months. Fluorotelomer alcohols were measured in headspace and parent monomers and all metabolites in soil extracts. Negligible degradation of FTU biodegradation occurred in the agricultural soil with 94 +/- 15% recovered at day 180. However, in the forest soil, both FTU and HMU degradation was evident with significant losses of 24% (117 d) and 27% (180 day), respectively, and concomitant increases in the terminal metabolite, perfluorooctanoic acid (PFOA) concentrations were well above what could result from residual 8:2 FTOH. Kinetic modeling estimated half-lives for FTU (aromatic backbone) and HMU (aliphatic backbone) in the forest soil to be 3-5 months and 15.9-22.2 months, respectively. The addition of a structurally similar non-fluorinated FTU analog, toluene-2,4-dicarbamic acid diethyl ester (TDAEE) enhanced production of terminal end products from 8:2 FTOH degradation. However, there was no clear evidence that TDAEE enhanced cleavage of the urethane bond, thus TDAEE appeared to just serve as an additional carbon source. TDAEE's half-life was approximately one week. A second addition of TDAEE appeared to retard subsequent degradation of FTU exemplifying the microbial dynamics and diversity impacting degradation of polyfluoroalkyl substances. Enhanced degradation of HMU was observed upon re-aeration indicating oxygen may have been limiting during some periods although degradation of intermediate metabolites to terminal metabolites was still occurring, albeit at slower rates.
CI - Copyright (c) 2015. Published by Elsevier Ltd.
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LA - eng
PT - Journal Article
DEP - 20151206
PL - England
TA - Chemosphere
JT - Chemosphere
JID - 0320657
SB - IM
OTO - NOTNLM
OT - Biotransformation

OT - Fluorotelomer urethane monomers
OT - PFOA
OT - Perfluoroalkyl substances
OT - Urethane cleavage
EDAT- 2015/12/02 06:00
MHDA- 2015/12/02 06:00
CRDT- 2015/12/02 06:00
PHST- 2015/05/08 [received]
PHST- 2015/10/16 [revised]
PHST- 2015/11/06 [accepted]
PHST- 2015/12/06 [aheadofprint]
AID - S0045-6535(15)30354-4 [pii]
AID - 10.1016/j.chemosphere.2015.11.021 [doi]
PST - ppublish
SO - Chemosphere. 2016 Feb;144:2482-8. doi: 10.1016/j.chemosphere.2015.11.021. Epub 2015 Dec 6.

PMID- 26745381
OWN - NLM
STAT- Publisher
DA - 20160108
LR - 20160109
IS - 1879-1298 (Electronic)
IS - 0045-6535 (Linking)
VI - 146
DP - 2015 Dec 30
TI - Electrochemical oxidation of perfluorinated compounds in water.
PG - 526-538
LID - S0045-6535(15)30446-X [pii]
LID - 10.1016/j.chemosphere.2015.11.115 [doi]
AB - Perfluorinated compounds (PFCs) are persistent and refractory organic pollutants that have been detected in various environmental matrices and municipal wastewater. Electrochemical oxidation (EO) is a promising remediation technique for wastewater contaminated with PFCs. A number of recent studies have demonstrated that the "non-active" anodes, including boron-doped diamond, tin oxide, and lead dioxide, are effective in PFCs elimination in wastewater due to their high oxygen evolution potential. Many researchers have conducted experiments to investigate the optimal conditions (i.e., potential, current density, pH value, plate distance, initial PFCs concentration, electrolyte, and other factors) for PFCs elimination to obtain the maximal elimination efficiency and current efficiency. The EO mechanism and pathways of PFCs have been clearly elucidated, which undergo electron transfer, Kolbe decarboxylation or desulfonation, hydrolysis, and radical reaction. In addition, the safety evaluation and energy consumption evaluation of the EO technology have also been summarized to decrease toxic ion release from electrode and reduce the cost of this technique. Although the ultrasonication and hydrothermal techniques combined with the EO process can improve the removal efficiency and current efficiency significantly, these coupled techniques have not been commercialized and applied

in industrial wastewater treatment. Finally, key challenges facing EO technology are listed and the directions for further research are pointed out (such as combination with other techniques, treatment for natural waters contaminated by low levels of PFCs, and reactor design).

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LA - ENG

PT - REVIEW

PT - JOURNAL ARTICLE

DEP - 20151230

TA - Chemosphere

JT - Chemosphere

JID - 0320657

OTO - NOTNLM

OT - Combination technique

OT - Electrochemical oxidation

OT - Electrochemical oxidation mechanisms

OT - Energy consumption

OT - Perfluorinated compounds

OT - Safety evaluation

EDAT- 2016/01/09 06:00

MHDA- 2016/01/09 06:00

CRDT- 2016/01/09 06:00

PHST- 2015/09/30 [received]

PHST- 2015/11/26 [revised]

PHST- 2015/11/27 [accepted]

AID - S0045-6535(15)30446-X [pii]

AID - 10.1016/j.chemosphere.2015.11.115 [doi]

PST - aheadofprint

SO - Chemosphere. 2015 Dec 30;146:526-538. doi: 10.1016/j.chemosphere.2015.11.115.

PMID- 26692515

OWN - NLM

STAT- Publisher

DA - 20151222

LR - 20151223

IS - 1879-1298 (Electronic)

IS - 0045-6535 (Linking)

VI - 145

DP - 2015 Dec 12

TI - Heat-activated persulfate oxidation of PFOA, 6:2 fluorotelomer sulfonate, and PFOS under conditions suitable for in-situ groundwater remediation.

PG - 376-383

LID - S0045-6535(15)30428-8 [pii]

LID - 10.1016/j.chemosphere.2015.11.097 [doi]

AB - PFOA (perfluorooctanoic acid) oxidation (0.121-6.04 μ M) by heat-activated persulfate was evaluated at 20-60 degrees C with 4.2-84 mM [Formula: see text] and in the presence of soluble fuel components to assess feasibility for in-situ remediation of groundwater. 6:2 fluorotelomer sulfonic acid/sulfonate (6:2 FTSA) and PFOS (perfluorooctanesulfonic acid) persulfate oxidation was also evaluated in a subset of conditions given their co-occurrence at many sites. High performance liquid chromatography electron spray tandem mass spectrometry was used for organic analysis and fluoride was measured using a fluoride-specific electrode. PFOA pseudo-1st order transformation rates (k_1 ,PFOA) increased with increasing temperature (half-lives from 0.1 to 7 d for 60 to 30 degrees C) sequentially removing CF₂ groups ('unzipping') to shorter chain perfluoroalkyl carboxylic acids (PFCAs) and F⁻. At 50 degrees C, a 5-fold increase in [Formula: see text] led to a 5-fold increase in k_1 ,PFOA after which self-scavenging by sulfate radicals decreased the relative rate of increase with more [Formula: see text] . Benzene, toluene, ethylbenzene and xylene did not affect k_1 ,PFOA even at 40 times higher molar concentrations than PFOA. A modeling approach to explore pathways strongly supported that for 6:2 FTSA, both the ethyl linkage and CF₂-CH₂ bond of 6:2 FTSA oxidize simultaneously, resulting in a ratio of approximately 25/75 PFHpA/PFHxA. The effectiveness of heat-activated [Formula: see text] on PFOA oxidation was reduced in a soil slurry; therefore, repeated persulfate injections are required to efficiently achieve complete oxidation in the field. However, PFOS remained unaltered even at higher activation temperatures, thus limiting the sole use of heat-activated persulfate for perfluoroalkyl substances removal in the field.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151212

TA - Chemosphere

JT - Chemosphere

JID - 0320657

OTO - NOTNLM

OT - 6:2 FTSA

OT - Heat-activated persulfate

OT - Oxidation

OT - PFOA

OT - PFOS

EDAT- 2015/12/23 06:00

MHDA- 2015/12/23 06:00

CRDT- 2015/12/23 06:00

PHST- 2015/07/01 [received]

PHST- 2015/11/24 [revised]

PHST- 2015/11/25 [accepted]

AID - S0045-6535(15)30428-8 [pii]

AID - 10.1016/j.chemosphere.2015.11.097 [doi]

PST - aheadofprint

SO - Chemosphere. 2015 Dec 12;145:376-383. doi: 10.1016/j.chemosphere.2015.11.097.

PMID- 26692511

OWN - NLM

STAT- Publisher

DA - 20151222

LR - 20151223

IS - 1879-1298 (Electronic)

IS - 0045-6535 (Linking)

VI - 145

DP - 2015 Dec 12

TI - Contribution of selected perfluoroalkyl and polyfluoroalkyl substances to the
adsorbable organically bound fluorine in German rivers and in a highly

contaminated groundwater.

PG - 342-350

LID - S0045-6535(15)30444-6 [pii]

LID - 10.1016/j.chemosphere.2015.11.113 [doi]

AB - Due to the lack of analytical standards the application of surrogate parameters for organofluorine detection in the aquatic environment is a complementary approach to single compound target analysis of perfluoroalkyl and polyfluoroalkyl chemicals (PFASs). The recently developed method adsorbable organically bound fluorine (AOF) is based on adsorption of organofluorine chemicals to activated carbon followed by combustion ion chromatography. This AOF method was further simplified to enable measurement of larger series of environmental samples. The limit of quantification (LOQ) was 0.77 µg/L F. The modified protocol was applied to 22 samples from German rivers, a municipal wastewater treatment plant (WWTP) effluent, and four groundwater samples from a fire-fighting training site. The WWTP effluent (AOF = 1.98 µg/L F) and only three river water samples (AOF between 0.88 µg/L F and 1.47 µg/L F) exceeded the LOQ. The AOF levels in a PFASs plume at a heavily contaminated site were in the range of 162 +/- 3 µg/L F to 782 +/- 43 µg/L F. In addition to AOF 17 PFASs were analyzed by high performance liquid chromatography-tandem mass spectrometry. 32-51% of AOF in the contaminated groundwater samples were explained by individual PFASs whereas in the surface waters more than 95% remained unknown. Organofluorine of two fluorinated pesticides, one pesticide metabolite and three fluorinated pharmaceuticals was recovered as AOF by >50% from all four tested water matrices. It is suggested that in the diffusely contaminated water bodies such fluorinated chemicals and not monitored PFASs contribute significantly to AOF.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151212

TA - Chemosphere

JT - Chemosphere

JID - 0320657

OTO - NOTNLM

OT - Adsorbable organically bound fluorine (AOF)

OT - Aqueous film forming foams (AFFFs)

OT - Combustion ion chromatography (CIC)
OT - Groundwater
OT - Perfluoroalkyl and polyfluoroalkyl substances (PFASs)
OT - Surface water
EDAT- 2015/12/23 06:00
MHDA- 2015/12/23 06:00
CRDT- 2015/12/23 06:00
PHST- 2015/08/19 [received]
PHST- 2015/11/26 [revised]
PHST- 2015/11/27 [accepted]
AID - S0045-6535(15)30444-6 [pii]
AID - 10.1016/j.chemosphere.2015.11.113 [doi]
PST - aheadofprint
SO - Chemosphere. 2015 Dec 12;145:342-350. doi: 10.1016/j.chemosphere.2015.11.113.

PMID- 26692506
OWN - NLM
STAT- Publisher
DA - 20151222
LR - 20151223
IS - 1879-1298 (Electronic)
IS - 0045-6535 (Linking)
VI - 145
DP - 2015 Dec 12
TI - A nuclear magnetic resonance study of the dynamics of organofluorine interactions with a dissolved humic acid.
PG - 307-313
LID - S0045-6535(15)30411-2 [pii]
LID - 10.1016/j.chemosphere.2015.11.080 [doi]
AB - A quantitative understanding of the dynamics of the interactions between organofluorine compounds and humic acids will contribute to an improved understanding of the role that Natural Organic Matter plays as a mediator in the fate, transport and distribution of these contaminants in the environment. Here, Nuclear Magnetic Resonance (NMR) spectroscopy-based diffusion measurements are used to estimate the association dynamics between dissolved humic acid and selected organofluorine compounds: pentafluoroaniline, pentafluorophenol, potassium perfluorooctane sulfonate, and perfluorooctanoic acid. Under the conditions used here, the strength of the association with humic acid increases linearly as temperature decreases for all compounds except for perfluorooctanoic acid, which exhibits divergent behavior with a non-linear decrease in the extent of interaction as temperature decreases. A general interaction mechanism controlled largely by desolvation effects is suggested for all compounds examined here except for perfluorooctanoic acid, which exhibits a specific mode of interaction consistent with a proteinaceous binding site. Reverse Heteronuclear Saturation Transfer Difference NMR is used to confirm the identity and nature of the humic acid binding sites.
CI - Copyright (c) 2015 Elsevier Ltd. All rights reserved.
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 LA - ENG
 PT - JOURNAL ARTICLE
 DEP - 20151212
 TA - Chemosphere
 JT - Chemosphere
 JID - 0320657
 OTO - NOTNLM
 OT - Association dynamics
 OT - Humic acid
 OT - Nuclear magnetic resonance
 OT - Organofluorine contaminants
 EDAT- 2015/12/23 06:00
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 PHST- 2015/09/23 [received]
 PHST- 2015/11/20 [revised]
 PHST- 2015/11/21 [accepted]
 AID - S0045-6535(15)30411-2 [pii]
 AID - 10.1016/j.chemosphere.2015.11.080 [doi]
 PST - aheadofprint
 SO - Chemosphere. 2015 Dec 12;145:307-313. doi: 10.1016/j.chemosphere.2015.11.080.

 PMID- 26172515
 OWN - NLM
 STAT- In-Process
 DA - 20151019
 IS - 1879-1298 (Electronic)
 IS - 0045-6535 (Linking)
 VI - 141
 DP - 2015 Dec
 TI - Electro-oxidation of perfluorooctanoic acid by carbon nanotube sponge anode and the mechanism.
 PG - 120-6
 LID - 10.1016/j.chemosphere.2015.06.095 [doi]
 LID - S0045-6535(15)00716-X [pii]
 AB - As an emerging persistent organic pollutant (POPs), perfluorooctanoic acid (PFOA) exists widely in natural environment. It is of particular significance to develop

efficient techniques to remove low-concentration PFOA from the contaminated waters. In this work, we adopted a new material, carbon nanotube (CNT) sponge, as electrode to enhance electro-oxidation and achieve high removal efficiency of low-concentration (100µg/L) PFOA from water. CNT sponge was pretreated by mixed acids to improve the surface morphology, hydrophilicity and the content of carbonyl groups on the surface. The highest removal efficiencies for low-concentration PFOA electrolyzed by acid-treated CNT sponge anode proved higher than 90%. The electro-oxidation mechanism of PFOA on CNT sponge anode was also discussed. PFOA is adsorbed on the CNT sponge rapidly increasing the concentration of PFOA on anode surface. When the potential on the anode is adjusted to more than 3.5V, the adsorbed PFOA undergoes electrochemically oxidation and hydrolysis to produce shorter-chain perfluorocarboxylic acids with less CF₂ unit. The efficient electro-oxidation of PFOA by CNT sponge anode is due to the combined effect of adsorption and electrochemical oxidation. These findings provide an efficient method to remove actual concentration PFOA from water.

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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

DEP - 20150711

PL - England

TA - Chemosphere

JT - Chemosphere
 JID - 0320657
 SB - IM
 OTO - NOTNLM
 OT - Adsorption
 OT - Carbon nanotube sponge
 OT - Electro-oxidation
 OT - Perfluorooctanoic acid (PFOA)
 EDAT- 2015/07/15 06:00
 MHDA- 2015/07/15 06:00
 CRDT- 2015/07/15 06:00
 PHST- 2015/05/04 [received]
 PHST- 2015/06/24 [revised]
 PHST- 2015/06/25 [accepted]
 PHST- 2015/07/11 [aheadofprint]
 AID - S0045-6535(15)00716-X [pii]
 AID - 10.1016/j.chemosphere.2015.06.095 [doi]
 PST - ppublish
 SO - Chemosphere. 2015 Dec;141:120-6. doi: 10.1016/j.chemosphere.2015.06.095. Epub 2015 Jul 11.

 PMID- 26764109
 OWN - NLM
 STAT- Publisher
 DA - 20160114
 LR - 20160115
 IS - 1873-4367 (Electronic)
 IS - 0927-7765 (Linking)
 VI - 140
 DP - 2015 Dec 31
 TI - Coating morphology and surface composition of acrylic terpolymers with pendant catechol, OEG and perfluoroalkyl groups in varying ratio and the effect on protein adsorption.
 PG - 254-261
 LID - S0927-7765(15)30399-4 [pii]
 LID - 10.1016/j.colsurfb.2015.12.051 [doi]
 AB - This work aims at developing versatile low-biofouling polymeric coatings by using acrylic terpolymers (DOFs) that bear pendant catechol (D), oligo(ethylene glycol) (O), and perfluoroalkyl (F) groups in varying ratios. The polymers were endowed with the ability to form firmly coatings on virtually any surfaces and undergo surface microphase separation and self-assembly, as revealed by the surface enrichment of F pendants and the morphology variation from irregular solid domains to discrete crater-type aggregates of different size. The effect on protein adsorption was investigated using bovine serum albumin (BSA) and adhesive fibrinogen (Fib) as model proteins. The coating of DOF164 (low F content), which has morphology of discrete crater-type aggregates of approximately 400nm in size, adsorbed a least amount of protein but with a highest protein unit activity as determined by SPR and immunosorbent assay; whereas the coating of DOF1612 (high F

content) showed a 12.3-fold higher adsorption capacity toward Fib. Interestingly, a 2.2-fold lower adsorption amount but with a 1.8-fold higher unit activity was found for Fib adsorbed on the DOF164 surface than on DOF250 (without F fraction), whose OEG segments being a widely recognized protein compatible material. The features of the DOF164 terpolymer presenting a robust coating ability and a minimal protein adsorption capacity while with a high protein unit activity suggest its potential application as a non-fouling surface-modifier for medical antifouling coatings and as a matrix material for selective protein immobilization and activity preservation in biosensor construction.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151231

TA - Colloids Surf B Biointerfaces

JT - Colloids and surfaces. B, Biointerfaces

JID - 9315133

OTO - NOTNLM

OT - Antifouling

OT - Catechol

OT - Dopamine

OT - Morphology

OT - Perfluoroalkyl

OT - Poly(ethylene glycol)

OT - Protein adsorption

OT - Terpolymer

EDAT- 2016/01/15 06:00

MHDA- 2016/01/15 06:00
 CRDT- 2016/01/15 06:00
 PHST- 2015/08/20 [received]
 PHST- 2015/12/03 [revised]
 PHST- 2015/12/27 [accepted]
 AID - S0927-7765(15)30399-4 [pii]
 AID - 10.1016/j.colsurfb.2015.12.051 [doi]
 PST - aheadofprint
 SO - Colloids Surf B Biointerfaces. 2015 Dec 31;140:254-261. doi:
 10.1016/j.colsurfb.2015.12.051.

PMID- 26403844
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151028
 IS - 2196-5412 (Electronic)
 VI - 2
 IP - 4
 DP - 2015 Dec
 TI - Maternal Exposure to Synthetic Chemicals and Obesity in the Offspring: Recent Findings.
 PG - 339-47
 LID - 10.1007/s40572-015-0068-6 [doi]
 AB - Experimental studies suggest perinatal exposures to synthetic chemicals may be associated with early onset obesity, although this hypothesis has not been extensively examined in humans. This article summarizes the evidence relating maternal perinatal exposure to common persistent organic compounds (polychlorinated biphenyl, dichlorodiphenyldichloroethylene, dichlorodiphenyltrichloroethane, hexachlorobenzene, hexachlorocyclohexane), perfluoroalkyls, perfluorooctane sulfonate, polybrominated diphenyl ethers and tributyltin, and nonpersistent compounds (phthalates, bisphenol A) on child obesity during sensitive developmental periods. Twenty-two epidemiologic studies published from 2011 to 2015 offer inconsistent support for the obesogenic effects of most substances and are limited by relatively small sample sizes and indirect measures of adiposity. The clearest findings suggest an influence of maternal dichlorodiphenyldichloroethylene exposure on offspring overweight and obesity. Recommendations for future epidemiological research include longer follow-up of effects of pre- and postnatal exposures in large samples; utilization of direct measures of adiposity; and consideration of effect modification by sex, birth weight, dietary fat, and maternal weight status.

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LA - eng

PT - Journal Article

PL - Switzerland

TA - Curr Environ Health Rep

JT - Current environmental health reports

JID - 101629387

SB - IM

OTO - NOTNLM

OT - Child

OT - Environmental obesogen

OT - Infant growth

OT - Maternal exposure

OT - Obesity

OT - Overweight

OT - Weight gain

EDAT- 2015/09/26 06:00

MHDA- 2015/09/26 06:00

CRDT- 2015/09/26 06:00

AID - 10.1007/s40572-015-0068-6 [doi]

AID - 10.1007/s40572-015-0068-6 [pii]

PST - ppublish

SO - Curr Environ Health Rep. 2015 Dec;2(4):339-47. doi: 10.1007/s40572-015-0068-6.

PMID- 26341623

OWN - NLM

STAT- In-Data-Review

DA - 20151028

LR - 20151031

IS - 2196-5412 (Electronic)

VI - 2

IP - 4

DP - 2015 Dec

TI - Cumulative Chemical Exposures During Pregnancy and Early Development.

PG - 367-78

LID - 10.1007/s40572-015-0064-x [doi]

AB - Industrial and consumer product chemicals are widely used, leading to ubiquitous human exposure to the most common classes. Because these chemicals may affect developmental milestones, exposures in pregnant women and developing fetuses are of particular interest. In this review, we discuss the prevalence of chemical exposures in pregnant women, the chemical class-specific relationships between maternal and fetal exposures, and the major sources of exposures for six chemical classes of concern: phthalates, phenols, perfluorinated compounds (PFCs), flame

retardants, polychlorinated biphenyls (PCBs), and organochlorine pesticides (OCs). Additionally, we describe the current efforts to characterize cumulative exposures to synthetic chemicals during pregnancy. We conclude by highlighting gaps in the literature and discussing possible applications of the findings to reduce the prevalence of cumulative exposures during pregnancy.

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LA - eng

GR - R00 ES019881/ES/NIEHS NIH HHS/United States

PT - Journal Article

PL - Switzerland

TA - Curr Environ Health Rep

JT - Current environmental health reports

JID - 101629387

SB - IM

PMC - PMC4626367

MID - NIHMS721246

OID - NLM: NIHMS721246 [Available on 12/01/16]

OID - NLM: PMC4626367 [Available on 12/01/16]

OTO - NOTNLM

OT - Cumulative exposure

OT - Flame retardants

OT - Organochlorine pesticides

OT - Perfluorinated compounds

OT - Phenols

OT - Phthalates

OT - Polychlorinated biphenyls

OT - Pregnancy

EDAT- 2015/09/06 06:00

MHDA- 2015/09/06 06:00

CRDT- 2015/09/06 06:00

PMCR- 2016/12/01 00:00

AID - 10.1007/s40572-015-0064-x [doi]

AID - 10.1007/s40572-015-0064-x [pii]

PST - ppublish

SO - Curr Environ Health Rep. 2015 Dec;2(4):367-78. doi: 10.1007/s40572-015-0064-x.

PMID- 26488228

OWN - NLM

STAT- In-Data-Review

DA - 20151114

IS - 1477-9234 (Electronic)

IS - 1477-9226 (Linking)

VI - 44

IP - 45

DP - 2015 Dec 7

TI - Approaches to prepare perfluoroalkyl and pentafluorophenyl copper couples for cross-coupling reactions with organohalogen compounds.

PG - 19693-9

LID - 10.1039/c5dt02925b [doi]

AB - The reactions of iodoperfluoroalkanes $C_nF_{2n+1}I$ ($n = 2, 3, 4$) and $n-BuLi$ at low temperatures give NMR spectroscopic evidence for LiC_nF_{2n+1} which were converted into $LiCu(C_nF_{2n+1})_2$ derivatives upon treatment with 0.5 mol copper(i) bromide, $CuBr$. An alternative route to obtain perfluoroorgano copper couples, $Cu(R_f)_2Ag$ ($R_f = n-C_3F_7, n-C_4F_9, C_6F_5$) was achieved from the reactions of the corresponding perfluoroorgano silver(i) reagents, AgR_f , and elemental copper through redox transmetallations. The composition of the resulting reactive intermediates was investigated by means of (^{19}F) NMR spectroscopy and ESI mass spectrometry. Perfluoro-*n*-propyl and perfluoro-*n*-butyl copper-silver reagents prepared by the oxidative transmetallation route exhibited good properties in C-C bond formation reactions with acid chlorides even under moderate conditions. Substitution of bromine directly bound to aromatics for perfluoroalkyl groups was achieved at elevated temperatures, while success in halide substitution reactions using lithium copper couples remained poor.

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FAU - Schafer, Mathias

AU - Schafer M

LA - eng

PT - Journal Article

DEP - 20151021

PL - England

TA - Dalton Trans

JT - Dalton transactions (Cambridge, England : 2003)
 JID - 101176026
 SB - IM
 EDAT- 2015/10/22 06:00
 MHDA- 2015/10/22 06:00
 CRDT- 2015/10/22 06:00
 PHST- 2015/10/21 [aheadofprint]
 PHST- 2015/11/10 [epublish]
 AID - 10.1039/c5dt02925b [doi]
 PST - ppublish
 SO - Dalton Trans. 2015 Dec 7;44(45):19693-9. doi: 10.1039/c5dt02925b. Epub 2015 Oct 21.

 PMID- 26473182
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151114
 IS - 1477-9234 (Electronic)
 IS - 1477-9226 (Linking)
 VI - 44
 IP - 45
 DP - 2015 Dec 7
 TI - Functionalization of Zr-based MOFs with alkyl and perfluoroalkyl groups: the effect on the water sorption behavior.
 PG - 19687-92
 LID - 10.1039/c5dt02908b [doi]
 AB - Stability and sorption of Metal-Organic Frameworks (MOFs) towards water are critical in many applications, and can a priori be modulated through the introduction of suitable organic functional groups on their backbone. We report here the preparation of a series of Zr(iv)-based MOFs functionalized with alkyl and perfluoroalkyl groups and their characterization by X-ray powder diffraction, multi-nuclei (¹H, ¹³C, ¹⁹F) solid state nuclear magnetic resonance analyses, and nitrogen sorption measurements at 77 K. Their water sorption behavior was evaluated at 298 K and related to their physico-chemical features, highlighting both the effect of the confinement and the nature of the functional groups on the hydrophilic/hydrophobic balance.
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 FAU - Bloch, E
 AU - Bloch E

FAU - Lavrard, H
 AU - Lavrard H
 FAU - Taulelle, F
 AU - Taulelle F
 FAU - Horcajada, P
 AU - Horcajada P
 FAU - Serre, C
 AU - Serre C
 FAU - Llewellyn, P L
 AU - Llewellyn PL
 FAU - Magnier, E
 AU - Magnier E
 FAU - Devic, T
 AU - Devic T
 LA - eng
 PT - Journal Article
 DEP - 20151016
 PL - England
 TA - Dalton Trans
 JT - Dalton transactions (Cambridge, England : 2003)
 JID - 101176026
 SB - IM
 EDAT- 2015/10/17 06:00
 MHDA- 2015/10/17 06:00
 CRDT- 2015/10/17 06:00
 PHST- 2015/10/16 [aheadofprint]
 PHST- 2015/11/10 [epublish]
 AID - 10.1039/c5dt02908b [doi]
 PST - ppublish
 SO - Dalton Trans. 2015 Dec 7;44(45):19687-92. doi: 10.1039/c5dt02908b. Epub 2015 Oct 16.

 PMID- 26459803
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151114
 IS - 1477-9234 (Electronic)
 IS - 1477-9226 (Linking)
 VI - 44
 IP - 45
 DP - 2015 Dec 7
 TI - Iron-catalyzed electrochemical C-H perfluoroalkylation of arenes.
 PG - 19674-81
 LID - 10.1039/c5dt03009a [doi]
 AB - A new iron-catalyzed reaction for the coupling of perfluoroalkyl iodides (RFI) with aromatic substrates is described. The perfluoroalkylated arene products are obtained in good to excellent yields in the presence of a [(bpy)Fe(ii)] catalyst (10%) electrochemically regenerated or generated from [(bpy)Fe(iii)] at room

temperature. The development, scope, and preliminary mechanistic studies of these transformations are reported.

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LA - eng

PT - Journal Article

DEP - 20151013

PL - England

TA - Dalton Trans

JT - Dalton transactions (Cambridge, England : 2003)

JID - 101176026

SB - IM

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PHST- 2015/11/10 [epublish]

AID - 10.1039/c5dt03009a [doi]

PST - ppublish

SO - Dalton Trans. 2015 Dec 7;44(45):19674-81. doi: 10.1039/c5dt03009a. Epub 2015 Oct 13.

PMID- 26440224
OWN - NLM
STAT- In-Data-Review
DA - 20151114
IS - 1477-9234 (Electronic)
IS - 1477-9226 (Linking)
VI - 44
IP - 45
DP - 2015 Dec 7
TI - Chemo-, regio-, and stereo-selective perfluoroalkylations by a Grignard complex with zirconocene.
PG - 19464-8
LID - 10.1039/c5dt03039k [doi]
AB - The synthesis of highly reactive perfluoroalkyl Grignard reagents with early transition metal zirconocene complexes and their new types of highly chemo-, regio-, and stereo-selective perfluoroalkylation reactions are reported with epoxides in particular. The zirconocene complex is advantageous in activating the perfluoroalkyl Grignard species. The zirconocene.Grignard complexes were clarified by DOSY. Both (1)H and (19)F DOSY analyses show that the addition of MAO and dioxane to the mixture of RFMgCl and Cp2ZrCl2 connects Cp2Zr and RFMg to generate the zirconocene/perfluoroalkyl-Grignard/dioxane complex.
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FAU - Mikami, Koichi
AU - Mikami K
LA - eng
PT - Journal Article
DEP - 20151006
PL - England
TA - Dalton Trans
JT - Dalton transactions (Cambridge, England : 2003)
JID - 101176026
SB - IM
EDAT- 2015/10/07 06:00
MHDA- 2015/10/07 06:00
CRDT- 2015/10/07 06:00
PHST- 2015/10/06 [aheadofprint]

PHST- 2015/11/10 [epublish]
 AID - 10.1039/c5dt03039k [doi]
 PST - ppublish
 SO - Dalton Trans. 2015 Dec 7;44(45):19464-8. doi: 10.1039/c5dt03039k. Epub 2015 Oct 6.

 PMID- 26374142
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151114
 IS - 1477-9234 (Electronic)
 IS - 1477-9226 (Linking)
 VI - 44
 IP - 45
 DP - 2015 Dec 7
 TI - Transition metal complexes bearing NHC ligands substituted with secondary polyfluoroalkyl groups.
 PG - 19663-73
 LID - 10.1039/c5dt02258d [doi]
 AB - Using three different approaches, racemic 1-(perfluoroalkyl)ethylamines were synthesized from perfluoroalkyl iodides or perfluoroalkanoic acids, and further transformed to the corresponding N,N'-disubstituted ethane-1,2-diimines and ethane-1,2-diamines as mixtures of diastereoisomers. Their cyclization afforded imidazolium or dihydroimidazolium salts, which led to silver or palladium complexes bearing NHC ligands substituted with secondary polyfluoroalkyl groups. The palladium complexes bearing a throwaway 3-chloropyridine ligand proved to be moderately active in the model Suzuki-Miyaura coupling.
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 FAU - Kvicala, J
 AU - Kvicala J
 LA - eng
 PT - Journal Article
 DEP - 20150916
 PL - England
 TA - Dalton Trans
 JT - Dalton transactions (Cambridge, England : 2003)
 JID - 101176026

SB - IM
 EDAT- 2015/09/17 06:00
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 PHST- 2015/11/10 [epublish]
 AID - 10.1039/c5dt02258d [doi]
 PST - ppublish
 SO - Dalton Trans. 2015 Dec 7;44(45):19663-73. doi: 10.1039/c5dt02258d. Epub 2015 Sep 16.

 PMID- 26211437
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151114
 IS - 1477-9234 (Electronic)
 IS - 1477-9226 (Linking)
 VI - 44
 IP - 45
 DP - 2015 Dec 7
 TI - Synthesis, structure, and reactivity of iridium perfluorocarbene complexes: regio- and stereo-specific addition of HCl across a metal carbon double bond.
 PG - 19528-42
 LID - 10.1039/c5dt02275d [doi]
 AB - Reductive activation of an alpha-fluorine in the perfluoroalkyl complexes Cp*(L)(i)Ir-CF2RF using Mg/graphite leads to perfluorocarbene complexes Cp*(L)Ir[double bond, length as m-dash]CFRF (L = CO, PMe3; RF = CF3, C2F5, C6F5). New complexes E-Cp*(PMe3)Ir[double bond, length as m-dash]CFC2F5 and E-Cp*(CO)Ir[double bond, length as m-dash]CFC6F5 have been characterized by single crystal X-ray diffraction studies, and a comparison of metric parameters with previously reported analogues is reported. Experimental NMR and computational DFT (B3LYP/LACV3P**++) studies agree that for Ir[double bond, length as m-dash]CFRF complexes (RF = CF3, CF2CF3) the thermodynamic preference for the E or Z isomer depends on the steric requirements of ligand L; when L = CO the Z-isomer (F cis to Cp*) is preferred and for L = PMe3 the E-isomer is preferred. When reduction of the precursors is carried out in the dark the reaction is completely selective to produce E- or Z-isomers. Exposure of solutions of these compounds to ambient light results in slow conversion to a photostationary non-equilibrium mixture of E and Z isomers. In the dark, these E/Z mixtures convert thermally to their preferred E or Z equilibrium geometries in an even slower reaction. A study of the temperature dependent kinetics of this dark transformation allows DeltaG(double dagger)298 for rotation about the Ir[double bond, length as m-dash]CFCF3 double bond to be experimentally determined as 25 kcal mol(-1); a DFT/B3LYP/LACV3P**++ calculation of this rotation barrier is in excellent agreement (27 kcal mol(-1)) with the experimental value. Reaction of HCl with toluene solutions of Cp*(L)Ir[double bond, length as m-dash]CFRF (L = CO, PMe3) or Cp*(CO)Ir[double bond, length as m-dash]C(CF3)2 at low temperature resulted in regiospecific addition of HCl

across the metal carbon double bond, ultimately yielding $\text{Cp}^*(\text{L})\text{Ir}(\text{CHFRF})\text{Cl}$ and $\text{Cp}^*(\text{CO})\text{Ir}[\text{CH}(\text{CF}_3)_2]\text{Cl}$. Reaction of HCl with single E or Z diastereomers of $\text{Cp}^*(\text{L})\text{Ir}[\text{double bond, length as m-dash}]\text{CFRF}$ gives stereospecific cis-addition to give single diastereomers of $\text{Cp}^*\text{Ir}(\text{L})(\text{CHFRF})\text{Cl}$; addition of HCl to several different E/Z ratios of $\text{Cp}^*(\text{L})\text{Ir}[\text{double bond, length as m-dash}]\text{CFRF}$ affords ratios of diastereomeric products $\text{Cp}^*(\text{L})\text{Ir}(\text{CHFRF})\text{Cl}$ identical to the original ratio of starting material isomers. The addition of HCl is therefore demonstrated to be unambiguously regio- and stereo-specific. The observed product regiochemistry of addition of HCl to $\text{Ir}[\text{double bond, length as m-dash}]\text{CF}_2$, $\text{Ir}[\text{double bond, length as m-dash}]\text{CFRF}$, and $\text{Ir}[\text{double bond, length as m-dash}]\text{C}(\text{CF}_3)_2$ ligands is the same and is not dependent on the ground state energy preference (singlet or triplet) for the free perfluorocarbene. DFT calculations on model HCl addition reactions indicate that this regiochemistry is strongly preferred thermodynamically, but predict that in $\text{H}(\delta^+)-\text{Cl}(\delta^-)$ addition to $\text{Cp}(\text{PH}_3)\text{Ir}[\text{double bond, length as m-dash}]\text{CF}_2$, $\text{H}(\delta^+)$ attack at Ir has a lower energy transition state, while for $\text{Cp}(\text{PH}_3)\text{Ir}[\text{double bond, length as m-dash}]\text{CFCF}_3$ and $\text{Cp}(\text{PH}_3)\text{Ir}[\text{double bond, length as m-dash}]\text{C}(\text{CF}_3)_2$, $\text{H}(\delta^+)$ attack at C is the kinetically preferred pathway. The carbene carbon atoms in $\text{Ir}[\text{double bond, length as m-dash}]\text{CFCF}_3$ and $\text{Ir}[\text{double bond, length as m-dash}]\text{C}(\text{CF}_3)_2$ complexes are unambiguously basic towards HCl , while in the $\text{Ir}[\text{double bond, length as m-dash}]\text{CF}_2$ analogues the carbene carbon is less basic than its Ir partner, and the eventual regiochemistry of HCl addition arises from thermodynamic control.

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AU - Hughes RP

LA - eng

PT - Journal Article

DEP - 20150727

PL - England

TA - Dalton Trans

JT - Dalton transactions (Cambridge, England : 2003)

JID - 101176026

SB - IM

EDAT- 2015/07/28 06:00

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PHST- 2015/07/27 [aheadofprint]

PHST- 2015/11/10 [epublish]

AID - 10.1039/c5dt02275d [doi]

PST - ppublish

SO - Dalton Trans. 2015 Dec 7;44(45):19528-42. doi: 10.1039/c5dt02275d. Epub 2015 Jul 27.

PMID- 26172122

OWN - NLM

STAT- In-Data-Review

DA - 20151114

IS - 1477-9234 (Electronic)

IS - 1477-9226 (Linking)

VI - 44

IP - 45

DP - 2015 Dec 7

TI - Polyfluorinated carba-closo-dodecaboranes with amino and ammonio substituents bonded to boron.

PG - 19576-86

LID - 10.1039/c5dt02055g [doi]

AB - The inner salts x-H3N-closo-1-CB11H11 (x = 12, 2) and 7-H3N-12-F-closo-1-CB11H11 were fluorinated with elemental fluorine in anhydrous hydrogen fluoride to give the B-perfluorinated ammonio derivatives 1-H-x-H3N-closo-1-CB11F10 (x = 12, 7, 2). Deprotonation of the ammonio group yielded the corresponding amino-functionalized anions [1-H-x-H2N-closo-1-CB11F10](-) (x = 12, 7, 2) that were isolated as [Et4N](+) salts. Hydrolysis of the highly fluorinated inner salts 1-H-x-H3N-closo-1-CB11F10 (x = 12, 7, 2) is very slow in acidic aqueous solutions. This stability of the ammonio derivatives is unprecedented because the related fluorinated anion [1-H2N-closo-1-CB11F11](-) is immediately hydrolyzed to simple boron species in the presence of aqueous acids. The ammonio derivatives 1-H-x-H3N-closo-1-CB11F10 (x = 12, 7, 2) are much more acidic compared to their non-fluorinated counterparts as assessed from potentiometric titrations and DFT calculations. The inner salts and the anions were characterized by NMR and vibrational spectroscopy. Solid-state structures of 1-H-12-H3N-closo-1-CB11F10.H2O, 1-H-7-H3N-closo-1-CB11F10.diglyme, 1-H-2-H3N-closo-1-CB11F10.0.5H2O, 7-H3N-12-F-closo-1-CB11H10.(CH3)2CO and [Et4N][1-H-12-H2N-closo-1-CB11F10] were determined by single-crystal X-ray diffraction.

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LA - eng

PT - Journal Article

DEP - 20150714
 PL - England
 TA - Dalton Trans
 JT - Dalton transactions (Cambridge, England : 2003)
 JID - 101176026
 SB - IM
 EDAT- 2015/07/15 06:00
 MHDA- 2015/07/15 06:00
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 PHST- 2015/07/14 [aheadofprint]
 PHST- 2015/11/10 [epublish]
 AID - 10.1039/c5dt02055g [doi]
 PST - ppublsh
 SO - Dalton Trans. 2015 Dec 7;44(45):19576-86. doi: 10.1039/c5dt02055g. Epub 2015 Jul 14.

 PMID- 26169553
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151114
 IS - 1477-9234 (Electronic)
 IS - 1477-9226 (Linking)
 VI - 44
 IP - 45
 DP - 2015 Dec 7
 TI - Gold trifluoromethyl complexes.
 PG - 19432-42
 LID - 10.1039/c5dt02023a [doi]
 AB - This article reviews the synthesis, reactivity and applications of gold trifluoromethyl complexes, which are the only isolated perfluoroalkyl complexes of gold. The most reported examples are neutral Au(i) complexes of the type [Au(CF₃)L], whereas only two Au(ii) trifluoromethyl complexes have been reported, both being diamagnetic and containing a strong Au-Au bond. A number of Au(iii) trifluoromethyl complexes have been prepared by oxidative addition of halogens or iodotrifluoromethane to Au(i) complexes or, in a few cases, by transmetallation reactions. Owing to the limitations of the available synthetic methods, a lower number of examples is known, particularly for the oxidation states (ii) and (iii). Gold trifluoromethyl complexes present singular characteristics, such as thermal stability, strong Au-C bonds and, in some cases, reactive alpha-C-F bonds. Some of the Au(iii) complexes reported, show unusually easy reductive elimination reactions of trifluoromethylated products which could be applied in the development of gold-catalyzed processes for the trifluoromethylation of organic compounds.
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 LA - eng
 PT - Journal Article
 DEP - 20150714
 PL - England
 TA - Dalton Trans
 JT - Dalton transactions (Cambridge, England : 2003)
 JID - 101176026
 SB - IM
 EDAT- 2015/07/15 06:00
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 CRDT- 2015/07/15 06:00
 PHST- 2015/07/14 [aheadofprint]
 PHST- 2015/11/10 [epublish]
 AID - 10.1039/c5dt02023a [doi]
 PST - ppublish
 SO - Dalton Trans. 2015 Dec 7;44(45):19432-42. doi: 10.1039/c5dt02023a. Epub 2015 Jul 14.

 PMID- 26158776
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151114
 IS - 1477-9234 (Electronic)
 IS - 1477-9226 (Linking)
 VI - 44
 IP - 45
 DP - 2015 Dec 7
 TI - A (pentafluoroethyl)(trifluoromethyl)carbene complex of iridium and reductive activation of its sp(3)alpha, beta, and gamma carbon-fluorine bonds to give perfluoro-2-butyne, perfluoro-1,2,3-butatriene and perfluoro-1-irida-2-methyl-2-cyclobutene) complexes.
 PG - 19518-27
 LID - 10.1039/c5dt02075a [doi]
 AB - The (pentafluoroethyl)(trifluoromethyl)carbene complex Cp*Ir(CO)[[double bond, length as m-dash]C(CF3)(C2F5)] was synthesized by the reductive activation of the alpha-C-F bond in the perfluoro-sec-butyl-iridium complex Cp*Ir(CO)[CF(CF3)(C2F5)](I) with Na/Pb alloy. This compound exists as two geometric isomers in solution; the structure of one isomer has been determined by a single crystal X-ray diffraction study and contains two independent molecules in the asymmetric unit. Further reduction of this carbene complex with Na/Pb alloy afforded the perfluoro-2-butyne iridium complex Cp*Ir(CO)(eta(2)-CF3C[triple bond, length as m-dash]CCF3) by an overall 2-electron reduction and elimination of two beta-fluorides. When magnesium graphite was utilized as the reducing agent for the further reduction, Cp*Ir(CO)(eta(2)-CF3C[triple bond, length as m-dash]CCF3) was produced as a minor product and the major product was the perfluoroiridacyclobutene complex Cp*Ir(CO)(eta(2,4)-CF3CCFCF2) resulting from a gamma-C-F bond activation. Direct

reduction of the precursor $\text{Cp}^*\text{Ir}(\text{CO})[\text{CF}(\text{CF}_3)(\text{C}_2\text{F}_5)](\text{i})$ with magnesium graphite generated the tetrafluorobutatriene iridium complex $\text{Cp}^*\text{Ir}(\text{CO})(\eta(2,3)\text{-CF}_2[\text{double bond, length as m-dash}]\text{C}[\text{double bond, length as m-dash}]\text{C}[\text{double bond, length as m-dash}]\text{CF}_2)$ along with the perfluoro-2-butyne complex and perfluoroiridacyclobutene complexes in a ratio of 1 : 2 : 6. These reductive inner-sphere pathways to unsaturated fluorocarbon ligands illustrate that carbon-fluorine bond activation can take place at α -, β - and γ -carbons but that selectivity in these heterogeneous reductions is difficult to control, with a variety of fluoride eliminations possible for complex perfluoroalkyl ligands. Density Functional Theory (DFT/B3LYP-D3/LACV3P**++) is used to explore the relative energetics of products and intermediates in these reactions.

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LA - eng

PT - Journal Article

DEP - 20150709

PL - England

TA - Dalton Trans

JT - Dalton transactions (Cambridge, England : 2003)

JID - 101176026

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PHST- 2015/11/10 [epublish]

AID - 10.1039/c5dt02075a [doi]

PST - ppublish

SO - Dalton Trans. 2015 Dec 7;44(45):19518-27. doi: 10.1039/c5dt02075a. Epub 2015 Jul 9.

PMID- 26034840

OWN - NLM

STAT- In-Data-Review

DA - 20151202

LR - 20151202

IS - 1552-9924 (Electronic)

IS - 0091-6765 (Linking)

VI - 123

IP - 12

DP - 2015 Dec

TI - Prenatal Exposure to Perfluoroalkyl Acids and Serum Testosterone Concentrations

at 15 Years of Age in Female ALSPAC Study Participants.

PG - 1325-30

LID - 10.1289/ehp.1408847 [doi]

AB - BACKGROUND: Exposure to perfluorooctane sulfonic acid (PFOS) or to perfluorooctanoic acid (PFOA) increases mouse and human peroxisome proliferator-activated receptor alpha (PPARalpha) subtype activity, which influences lipid metabolism. Because cholesterol is the substrate from which testosterone is synthesized, exposure to these substances has the potential to alter testosterone concentrations. OBJECTIVES: We explored associations of total testosterone and sex hormone-binding globulin (SHBG) concentrations at age 15 years with prenatal exposures to PFOS, PFOA, perfluorohexane sulfonic acid (PFHxS), and perfluoronanoic acid (PFNA) in females. METHODS: Prenatal concentrations of the perfluoroalkyl acids (PFAAs) were measured in serum collected from pregnant mothers at enrollment (1991-1992) in the Avon Longitudinal Study of Parents and Children (ALSPAC). The median gestational age when the maternal blood sample was obtained was 16 weeks (interquartile range, 11-28 weeks). Total testosterone and SHBG concentrations were measured in serum obtained from their daughters at 15 years of age. Associations between prenatal PFAAs concentrations and reproductive outcomes were estimated using linear regression models (n = 72). RESULTS: Adjusted total testosterone concentrations were on average 0.18-nmol/L (95% CI: 0.01, 0.35) higher in daughters with prenatal PFOS in the upper concentration tertile compared with daughters with prenatal PFOS in the lower tertile. Adjusted total testosterone concentrations were also higher in daughters with prenatal concentrations of PFOA (beta = 0.24; 95% CI: 0.05, 0.43) and PFHxS (beta = 0.18; 95% CI: 0.00, 0.35) in the upper tertile compared with daughters with concentrations in the lower tertile. We did not find evidence of associations between PFNA and total testosterone or between any of the PFAAs and SHBG. CONCLUSIONS: Our findings were based on a small study sample and should be interpreted with caution. However, they suggest that prenatal exposure to some PFAAs may alter testosterone concentrations in females. CITATION: Maisonet M, Calafat AM, Marcus M, Jaakkola JJ, Lashen H. 2015. Prenatal exposure to perfluoroalkyl acids and serum testosterone concentrations at 15 years of age in female ALSPAC study participants. Environ Health Perspect 123:1325-1330; <http://dx.doi.org/10.1289/ehp.1408847>.

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FAU - Jaakkola, Jouni J K

AU - Jaakkola JJ

FAU - Lashen, Hany

AU - Lashen H

LA - eng

GR - 102215/Wellcome Trust/United Kingdom

PT - Journal Article
DEP - 20150602
PL - United States
TA - Environ Health Perspect
JT - Environmental health perspectives
JID - 0330411
SB - IM
PMC - PMC4671244
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PHST- 2015/05/28 [accepted]
PHST- 2015/06/02 [aheadofprint]
AID - 10.1289/ehp.1408847 [doi]
PST - ppublish
SO - Environ Health Perspect. 2015 Dec;123(12):1325-30. doi: 10.1289/ehp.1408847. Epub 2015 Jun 2.

PMID- 26008903
OWN - NLM
STAT- In-Data-Review
DA - 20151202
IS - 1552-9924 (Electronic)
IS - 0091-6765 (Linking)
VI - 123
IP - 12
DP - 2015 Dec
TI - Associations of Perfluoroalkyl Substances (PFAS) with Lower Birth Weight: An Evaluation of Potential Confounding by Glomerular Filtration Rate Using a Physiologically Based Pharmacokinetic Model (PBPK).
PG - 1317-24
LID - 10.1289/ehp.1408837 [doi]
AB - BACKGROUND: Prenatal exposure to perfluoroalkyl substances (PFAS) has been associated with lower birth weight in epidemiologic studies. This association could be attributable to glomerular filtration rate (GFR), which is related to PFAS concentration and birth weight. OBJECTIVES: We used a physiologically based pharmacokinetic (PBPK) model of pregnancy to assess how much of the PFAS-birth weight association observed in epidemiologic studies might be attributable to GFR. METHODS: We modified a PBPK model to reflect the association of GFR with birth weight (estimated from three studies of GFR and birth weight) and used it to simulate PFAS concentrations in maternal and cord plasma. The model was run 250,000 times, with variation in parameters, to simulate a population. Simulated data were analyzed to evaluate the association between PFAS levels and birth weight due to GFR. We compared simulated estimates with those from a meta-analysis of epidemiologic data. RESULTS: The reduction in birth weight for each 1-ng/mL increase in simulated cord plasma for perfluorooctane sulfonate (PFOS) was 2.72 g (95% CI: -3.40, -2.04), and for perfluorooctanoic acid (PFOA)

was 7.13 g (95% CI: -8.46, -5.80); results based on maternal plasma at term were similar. Results were sensitive to variations in PFAS level distributions and the strength of the GFR-birth weight association. In comparison, our meta-analysis of epidemiologic studies suggested that each 1-ng/mL increase in prenatal PFOS and PFOA levels was associated with 5.00 g (95% CI: -21.66, -7.78) and 14.72 g (95% CI: -8.92, -1.09) reductions in birth weight, respectively. CONCLUSION: Results of our simulations suggest that a substantial proportion of the association between prenatal PFAS and birth weight may be attributable to confounding by GFR and that confounding by GFR may be more important in studies with sample collection later in pregnancy. CITATION: Verner MA, Loccisano AE, Morken NH, Yoon M, Wu H, McDougall R, Maisonet M, Marcus M, Kishi R, Miyashita C, Chen MH, Hsieh WS, Andersen ME, Clewell HJ III, Longnecker MP. 2015. Associations of perfluoroalkyl substances (PFAS) with lower birth weight: an evaluation of potential confounding by glomerular filtration rate using a physiologically based pharmacokinetic model (PBPk). Environ Health Perspect 123:1317-1324; <http://dx.doi.org/10.1289/ehp.1408837>.

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AU - Longnecker MP

LA - eng
 PT - Journal Article
 DEP - 20150522
 PL - United States
 TA - Environ Health Perspect
 JT - Environmental health perspectives
 JID - 0330411
 SB - IM
 PMC - PMC4671243
 EDAT- 2015/05/27 06:00
 MHDA- 2015/05/27 06:00
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 PHST- 2015/05/22 [aheadofprint]
 AID - 10.1289/ehp.1408837 [doi]
 PST - ppublish
 SO - Environ Health Perspect. 2015 Dec;123(12):1317-24. doi: 10.1289/ehp.1408837. Epub 2015 May 22.

 PMID- 26722671
 OWN - NLM
 STAT- Publisher
 DA - 20160101
 LR - 20160102
 IS - 1873-6750 (Electronic)
 IS - 0160-4120 (Linking)
 VI - 88
 DP - 2015 Dec 23
 TI - Perfluoroalkyl substances and food allergies in adolescents.
 PG - 74-79
 LID - S0160-4120(15)30122-7 [pii]
 LID - 10.1016/j.envint.2015.12.020 [doi]
 AB - Perfluoroalkyl and polyfluoroalkyl substances (PFASs) are a class of organic compounds that are persistent in the environment due to their stable carbon-fluorine backbone, which is not susceptible to degradation. Research suggests these chemicals may exert an immunotoxic effect. The aim of this study is to investigate the associations between four PFASs - perfluorooctane sulfonic acid (PFOS), perfluorooctanoic acid (PFOA), perfluorononanoic acid (PFNA), and perfluorohexane sulfonic acid (PFHxS) - with food sensitization and food allergies in adolescent participants (ages 12-19years) in the National Health and Nutrition Examination Survey (NHANES) 2005-2006 and 2007-2010, respectively. We performed multivariate logistic regression to analyze the association between individual PFASs with food sensitization (defined as having at least 1 food-specific IgE level ≥ 0.35 kU/L) in NHANES 2005-2006 and food allergies (self-reported) in NHANES 2007-2010. Serum PFOA, PFOS, and PFHxS were statistically significantly associated with higher odds to have self-reported food allergies in NHANES 2007-2010. When using IgE levels as a marker of food

sensitization, we found that serum PFNA was inversely associated with food sensitization (NHANES 2005-2006). In conclusion, we found that serum levels of PFASs were associated with higher odds to have self-reported food allergies. Conversely, adolescents with higher serum PFNA were less likely to be sensitized to food allergens. These results, along with previous studies, warrant further investigation, such as well-designed longitudinal studies.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151223

TA - Environ Int

JT - Environment international

JID - 7807270

OTO - NOTNLM

OT - Adolescents

OT - Food allergies

OT - NHANES

OT - Perfluoroalkyl compounds

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PST - aheadofprint

SO - Environ Int. 2015 Dec 23;88:74-79. doi: 10.1016/j.envint.2015.12.020.

PMID- 26700417

OWN - NLM

STAT- Publisher

DA - 20151224

LR - 20151225

IS - 1873-6750 (Electronic)

IS - 0160-4120 (Linking)

VI - 88

DP - 2015 Dec 14

TI - Serum perfluorinated chemicals, glucose homeostasis and the risk of diabetes in

working-aged Taiwanese adults.

PG - 15-22

LID - S0160-4120(15)30100-8 [pii]

LID - 10.1016/j.envint.2015.11.016 [doi]

AB - BACKGROUND: The link among perfluoroalkyl and polyfluoroalkyl substances (PFASs), abnormal glucose homeostasis and the risk of diabetes has been intensively debated with conflicting evidence. OBJECTIVES: We evaluated the associations among PFASs, oral glucose tolerance testing (OGTT) curves and diabetes prevalence in 571 working-aged Taiwanese participants. METHODS: Exposure measures included serum perfluorooctanoic acid (PFOA), perfluorooctane sulfonic acid (PFOS), perfluorononanoic acid (PFNA), and perfluoroundecanoic acid (PFUA). Outcomes were OGTT curves and prevalent diabetes defined by fasting blood glucose (FBG) ≥ 126 mg/dL, 2-h glucose ≥ 200 mg/dL, or glycated hemoglobin $\geq 6.5\%$. Analyses were performed with multiple logistic regression and functional data analysis. RESULTS: A total of 39 participants (6.8%) had diabetes in this study. After full adjustment, the increase in the geometric means of FBG, 2-h glucose concentrations, and area under the OGTT curve (AUC₁₂₀) with a doubling increase in PFOS was 3% (95% CI 1-4), 8% (5-12), and 6% (4-9), respectively. Compared to the lowest-quartile of PFOS concentrations (<2.4 ng/ml), the OGTT trajectories were significantly steeper in participants of the highest-quartile PFOS exposure (>4.8 ng/ml) and the vertical shifting of the mean curve for each PFOS quartile showed a dose-response pattern. The adjusted odds ratio for diabetes comparing the highest to lowest quartile was 3.37 (95% CI 1.18-9.65). For PFOA, PFNA, and PFUA, the opposite pattern of OGTT trajectory and the opposite risk profile for diabetes were observed. CONCLUSIONS: Chronic PFOS exposure was associated with impaired glucose homeostasis and the increased prevalence of diabetes. However, PFOA, PFNA, and PFUA showed a potential protective effect against glucose intolerance and the risk of diabetes. Future research focusing on clarifying possible differential effects of different species of PFASs on glucose homeostasis and establishing the prospective associations between PFASs and diabetes is needed.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151214

TA - Environ Int

JT - Environment international

JID - 7807270

OTO - NOTNLM

OT - Diabetes

OT - Glucose homeostasis

OT - Oral glucose tolerance testing

OT - Perfluorinated chemicals

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SO - Environ Int. 2015 Dec 14;88:15-22. doi: 10.1016/j.envint.2015.11.016.

PMID- 26298835

OWN - NLM

STAT- In-Data-Review

DA - 20151116

IS - 1873-6750 (Electronic)

IS - 0160-4120 (Linking)

VI - 85

DP - 2015 Dec

TI - Exploring the fate, transport and risk of Perfluorooctane Sulfonate (PFOS) in a

coastal region of China using a multimedia model.

PG - 15-26

LID - 10.1016/j.envint.2015.08.007 [doi]

LID - S0160-4120(15)30035-0 [pii]

AB - Perfluorooctane Sulfonate (PFOS) and related substances have been widely applied in both industrial processes and domestic products in China. Exploring the environmental fate and transport of PFOS using modeling methods provides an important link between emission and multimedia diffusion which forms a vital part in the human health risk assessment and chemical management for these substances. In this study, the gridded fugacity based BETR model was modified to make it more suitable to model transfer processes of PFOS in a coastal region, including changes to PFOS partition coefficients to reflect the influence of water salinity on its sorption behavior. The fate and transport of PFOS in the Bohai coastal region of China were simulated under steady state with the modified version of the model. Spatially distributed emissions of PFOS and related substances in 2010 were estimated and used in these simulations. Four different emission scenarios were investigated, in which a range of half-lives for PFOS related substances were considered. Concentrations of PFOS in air, vegetation, soil, fresh water, fresh water sediment and coastal water were derived from the model under the steady-state assumption. The median modeled PFOS concentrations in fresh water, fresh water sediment and soil were 7.20ng/L, 0.39ng/g and 0.21ng/g, respectively, under Emission Scenario 2 (which assumed all PFOS related substances immediately degrade to PFOS) for the whole region, while the maximum concentrations were 47.10ng/L, 4.98ng/g and 2.49ng/g, respectively. Measured concentration data for PFOS in the Bohai coastal region around the year of 2010 were collected from the literature. The reliability of the model results was evaluated by comparing the range of modeled concentrations with the measured data, which generally matched well for the main compartments. Fate and transfer fluxes were derived from the model based on the calculated inventory within the compartments, transfer fluxes between compartments and advection fluxes between sub-regions. It showed that soil and coastal water were likely to be the most important sinks of PFOS in the Bohai coastal region, in which more than 90% of PFOS was stored. Flows of fresh water were the driving force for spatial transport of PFOS in this region. Influences of the seasonal change of fresh water fluxes on the model results were also analyzed. When only seasonal changes of the fresh water flow rates were considered, concentrations of PFOS in winter and spring were predicted to be higher than that under annual average conditions, while the concentrations in summer and autumn were lower. For PFOS fluxes entering the sea, opposite conclusions were drawn compared to the concentrations. Environmental risks from the presence of PFOS in fresh water were assessed for this region through comparison with available water quality criteria values. The predicted concentrations of PFOS in the Bohai coastal region provided by the model were lower than the water quality criteria published by the United States Environmental Protection Agency and Chinese researchers, while the concentrations in more than 80% of the sampling locations exceeded the European Union Water Framework Directive Environmental Quality Standards values. Seasonal variations of flow rate might cause a significant increase in environmental risks.

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LA - eng
PT - Journal Article
DEP - 20150824
PL - Netherlands
TA - Environ Int
JT - Environment international
JID - 7807270
SB - IM
OTO - NOTNLM
OT - Bohai coastal region
OT - Environmental risk
OT - Fugacity based gridded model
OT - Multimedia transportation
OT - Perfluorooctane Sulfonate (PFOS)
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PST - ppublish

SO - Environ Int. 2015 Dec;85:15-26. doi: 10.1016/j.envint.2015.08.007. Epub 2015 Aug 24.

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OWN - NLM

STAT- Publisher

DA - 20160108

LR - 20160109

IS - 1873-6424 (Electronic)

IS - 0269-7491 (Linking)

VI - 211

DP - 2015 Dec 30

TI - Perfluorinated compounds in soil, surface water, and groundwater from rural areas in eastern China.

PG - 124-131

LID - S0269-7491(15)30238-4 [pii]

LID - 10.1016/j.envpol.2015.12.024 [doi]

AB - Little research on perfluorinated compounds (PFCs) has been conducted in rural areas, although rural PFC sources are less complicated than in urban and industrial areas. To determine the levels and geographical distribution of 17 PFC compounds, samples of soil, surface water, and groundwater were collected from eight rural areas in eastern China. The total PFC concentrations (summation operatorPFCs) in soils ranged from 0.34 to 65.8 ng/g summation operatorPFCs in surface waters ranged from 7.0 to 489 ng/L and summation operatorPFCs in groundwater ranged from 5.3 to 615 ng/L. Ratios of perfluorononanoic acid/perfluorooctanoic acid (PFNA/PFOA), perfluoro-n-butyric acid/perfluorooctanoic acid (PFBA/PFOA), and perfluoroheptanoic acid/perfluorooctanoic acid (PFHpA/PFOA) in rainwater increased due to the fluorine chemical plants in the surrounding rural and urban areas, suggesting that atmospheric precipitation may carry PFCs and their precursors from the fluorochemical industrial area to the adjacent rural areas.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151230

TA - Environ Pollut

JT - Environmental pollution (Barking, Essex : 1987)

JID - 8804476

OTO - NOTNLM

OT - Eastern China

OT - Groundwater

OT - PFCs

OT - Rural areas

OT - Soil

OT - Surface water

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AID - 10.1016/j.envpol.2015.12.024 [doi]

PST - aheadofprint

SO - Environ Pollut. 2015 Dec 30;211:124-131. doi: 10.1016/j.envpol.2015.12.024.

PMID- 26367703

OWN - NLM

STAT- In-Data-Review

DA - 20151125

IS - 1873-6424 (Electronic)

IS - 0269-7491 (Linking)

VI - 207

DP - 2015 Dec

TI - Estimating emissions of PFOS and PFOA to the Danube River catchment and evaluating them using a catchment-scale chemical transport and fate model.

PG - 97-106

LID - 10.1016/j.envpol.2015.08.050 [doi]

LID - S0269-7491(15)30044-0 [pii]

AB - Novel approaches for estimating the emissions of perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) to surface waters are explored. The Danube River catchment is used to investigate emissions contributing to riverine loads of PFOS and PFOA and to verify the accuracy of estimates using a catchment-scale dynamic fugacity-based chemical transport and fate model (STREAM-EU; Spatially and Temporally Resolved Exposure Assessment Model for European basins). Model accuracy evaluation performed by comparing STREAM-EU predicted concentrations and monitoring data for the Danube and its tributaries shows that the best estimates for PFOS and PFOA emissions in the Danube region are obtained by considering the combined contributions of human population, wealth (based on local gross domestic product (GDP)) and wastewater treatment. Human population alone cannot explain the levels of PFOS and PFOA found in the Danube catchment waters. Introducing wealth distribution information in the form of local GDPs improves emission estimates markedly, likely by better representing emissions resulting from consumer trends, industrial and commercial sources. For compounds such as PFOS and PFOA, whose main sink and transport media is the aquatic compartment, a major source to freshwater are wastewater treatment plants. Introducing wastewater treatment information in the emission estimations also further improves emission estimates.

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LA - eng

PT - Journal Article

DEP - 20150911

PL - England

TA - Environ Pollut

JT - Environmental pollution (Barking, Essex : 1987)
 JID - 8804476
 SB - IM
 OTO - NOTNLM
 OT - Danube basin
 OT - Emissions estimation
 OT - Modelling
 OT - PFOA
 OT - PFOS
 EDAT- 2015/09/15 06:00
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 AID - S0269-7491(15)30044-0 [pii]
 AID - 10.1016/j.envpol.2015.08.050 [doi]
 PST - ppublish
 SO - Environ Pollut. 2015 Dec;207:97-106. doi: 10.1016/j.envpol.2015.08.050. Epub 2015 Sep 11.

 PMID- 26656511
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160107
 IS - 1096-0953 (Electronic)
 IS - 0013-9351 (Linking)
 VI - 145
 DP - 2016 Feb
 TI - Carcinogenicity of consumption of red and processed meat: What about environmental contaminants?
 PG - 109-15
 LID - 10.1016/j.envres.2015.11.031 [doi]
 LID - S0013-9351(15)30159-6 [pii]
 AB - In October 26, 2015, the International Agency for Research on Cancer (IARC) issued a press release informing of the recent evaluation of the carcinogenicity of red and processed meat consumption. The consumption of red meat and processed meat was classified as "probably carcinogenic to humans", and as "carcinogenic to humans", respectively. The substances responsible of this potential carcinogenicity would be generated during meat processing, such as curing and smoking, or when meat is heated at high temperatures (N-nitroso-compounds, polycyclic aromatic hydrocarbons and heterocyclic aromatic amines). However, in its assessments, the IARC did not make any reference to the role that may pose some carcinogenic environmental pollutants, which are already present in raw or unprocessed meat. The potential role of a number of environmental chemical contaminants (toxic trace elements, polycyclic aromatic hydrocarbons, polychlorinated dibenzo-p-dioxins and dibenzofurans, polychlorinated biphenyls,

polybrominated diphenyl ethers, polychlorinated diphenyl ethers, polychlorinated naphthalenes and perfluoroalkyl substances) on the carcinogenicity of consumption of meat and meat products is discussed in this paper. A case-study, Catalonia (Spain), is specifically assessed, while the influence of cooking on the concentrations of environmental pollutants is also reviewed. It is concluded that although certain cooking processes could modify the levels of chemical contaminants in food, the influence of cooking on the pollutant concentrations depends not only on the particular cooking process, but even more on their original contents in each specific food item. As most of these environmental pollutants are organic, cooking procedures that release or remove fat from the meat should tend to reduce the total concentrations of these contaminants in the cooked meat.

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LA - eng

PT - Journal Article

DEP - 20151206

PL - United States

TA - Environ Res

JT - Environmental research

JID - 0147621

SB - IM

OTO - NOTNLM

OT - Carcinogenicity

OT - Cooking

OT - Dietary exposure

OT - Environmental contaminants

OT - Meat and meat products

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SO - Environ Res. 2016 Feb;145:109-15. doi: 10.1016/j.envres.2015.11.031. Epub 2015 Dec 6.

PMID- 26656498

OWN - NLM

STAT- In-Data-Review

DA - 20160107

IS - 1096-0953 (Electronic)

IS - 0013-9351 (Linking)

VI - 145

DP - 2016 Feb

TI - Perfluorooctanoic acid and chronic kidney disease: Longitudinal analysis of a Mid-Ohio Valley community.

PG - 85-92

LID - 10.1016/j.envres.2015.11.018 [doi]

LID - S0013-9351(15)30146-8 [pii]

AB - INTRODUCTION: Perfluorooctanoic acid (PFOA) is an environmentally persistent chemical found at low-levels in the serum of almost all U.S. residents. Chronic kidney disease (CKD) has been positively associated with serum PFOA in prior cross-sectional studies and in one occupational mortality study, while other investigations have found no association between kidney function and PFOA. METHODS: We conducted a longitudinal analysis of chronic kidney disease among adults, aged ≥ 20 years, (N=32,254) in a Mid-Ohio Valley community cohort, exposed to high PFOA levels from contaminated drinking water. Estimated retrospective yearly serum PFOA concentrations (1951-2011) were previously modeled in this population. Information about lifetime history of CKD diagnosis was collected during surveys in 2008-2011; self-reported CKD diagnoses were validated through medical record review. Using a Cox proportional hazards model, we retrospectively examined the association between validated adult onset CKD, and modeled PFOA exposure, from time of first exposure. We also analyzed data for the cohort prospectively, among people with no CKD diagnosis prior to enrollment in a baseline survey in 2005-2006. Both the full cohort and a non-diabetic subset were analyzed, retrospectively and prospectively. RESULTS: Neither in retrospective nor in prospective analyses did we find a significant ($\alpha=0.05$) trend between PFOA exposure and CKD. In the full cohort, estimated hazard ratios by quintile of cumulative serum PFOA in the retrospective analysis were 1.00 (referent), 1.26, 1.12, 1.12 and 1.24 (trend test for log cumulative exposure: $p=0.80$). CONCLUSION: Our analyses suggest that CKD is not associated with exposure to PFOA.

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LA - eng
PT - Journal Article
DEP - 20151206
PL - United States
TA - Environ Res
JT - Environmental research
JID - 0147621
SB - IM
OTO - NOTNLM
OT - Chronic kidney disease
OT - Cohort
OT - Longitudinal
OT - Perfluorooctanoic acid
EDAT- 2015/12/15 06:00
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PHST- 2015/11/04 [revised]
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PHST- 2015/12/06 [aheadofprint]
AID - S0013-9351(15)30146-8 [pii]
AID - 10.1016/j.envres.2015.11.018 [doi]
PST - ppublish
SO - Environ Res. 2016 Feb;145:85-92. doi: 10.1016/j.envres.2015.11.018. Epub 2015 Dec
6.

PMID- 26636352
OWN - NLM
STAT- In-Data-Review

DA - 20160105
 IS - 1520-5851 (Electronic)
 IS - 0013-936X (Linking)
 VI - 50
 IP - 1
 DP - 2016 Jan 5
 TI - Perfluoroalkyl Acids Inhibit Reductive Dechlorination of Trichloroethene by Repressing Dehalococcoides.
 PG - 240-8
 LID - 10.1021/acs.est.5b04854 [doi]
 AB - The subsurface recalcitrance of perfluoroalkyl acids (PFAAs) derived from aqueous film-forming foams could have adverse impacts on the microbiological processes used for the bioremediation of co-mingled chlorinated solvents such as trichloroethene (TCE). Here, we show that reductive dechlorination by a methanogenic, mixed culture was significantly inhibited when exposed to concentrations representative of PFAA source zones (>66 mg/L total of 11 PFAA analytes, 6 mg/L each). TCE dechlorination, cis-dichloroethene and vinyl chloride production and dechlorination, and ethene generation were all inhibited at these PFAA concentrations. Phylogenetic analysis revealed that the abundances of 65% of the operational taxonomic units (OTUs) changed significantly when grown in the presence of PFAAs, although repression or enhancement resulting from PFAA exposure did not correlate with putative function or phylogeny. Notably, there was significant repression of Dehalococcoides (8-fold decrease in abundance) coupled with a corresponding enhancement of methane-generating Archaea (a 9-fold increase). Growth and dechlorination by axenic cultures of Dehalococcoides mccartyi strain 195 were similarly repressed under these conditions, confirming an inhibitory response of this pivotal genus to PFAA presence. These results suggest that chlorinated solvent bioattenuation rates could be impeded in subsurface environments near PFAA source zones.
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 LA - eng
 PT - Journal Article
 DEP - 20151221
 PL - United States
 TA - Environ Sci Technol
 JT - Environmental science & technology
 JID - 0213155
 SB - IM
 EDAT- 2015/12/05 06:00
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 AID - 10.1021/acs.est.5b04854 [doi]
 PST - ppublish
 SO - Environ Sci Technol. 2016 Jan 5;50(1):240-8. doi: 10.1021/acs.est.5b04854. Epub 2015 Dec 21.

 PMID- 26686982
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160119
 IS - 1520-5851 (Electronic)
 IS - 0013-936X (Linking)
 VI - 50
 IP - 2
 DP - 2016 Jan 19
 TI - Perfluorooctanoic Acid Degradation Using UV-Persulfate Process: Modeling of the Degradation and Chlorate Formation.
 PG - 772-81
 LID - 10.1021/acs.est.5b03715 [doi]
 AB - In this study, we investigated the destruction and by-product formation of perfluorooctanoic acid (PFOA) using ultraviolet light and persulfate (UV-PS). Additionally, we developed a first-principles kinetic model to simulate both PFOA destruction and by-product and chlorate (ClO₃(-)) formation in ultrapure water (UW), surface water (SW), and wastewater (WW). PFOA degradation was significantly suppressed in the presence of chloride and carbonate species and did not occur until all the chloride was converted to ClO₃(-) in UW and for low DOC concentrations in SW. The model was able to simulate the PS decay, pH changes, radical concentrations, and ClO₃(-) formation for UW and SW. However, our model was unable to simulate PFOA degradation well in WW, possibly from PS activation by NOM, which in turn produced sulfate radicals.
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PT - Journal Article

DEP - 20151230

PL - United States

TA - Environ Sci Technol

JT - Environmental science & technology

JID - 0213155

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EDAT- 2015/12/22 06:00

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AID - 10.1021/acs.est.5b03715 [doi]

PST - ppublish

SO - Environ Sci Technol. 2016 Jan 19;50(2):772-81. doi: 10.1021/acs.est.5b03715. Epub 2015 Dec 30.

PMID- 26653085

OWN - NLM

STAT- In-Data-Review

DA - 20160119

IS - 1520-5851 (Electronic)

IS - 0013-936X (Linking)

VI - 50

IP - 2

DP - 2016 Jan 19

TI - Is Ongoing Sulfluramid Use in South America a Significant Source of Perfluorooctanesulfonate (PFOS)? Production Inventories, Environmental Fate, and Local Occurrence.

PG - 653-9

LID - 10.1021/acs.est.5b04544 [doi]

AB - Despite international phase-out initiatives, production and use of perfluorooctanesulfonate (PFOS) and related substances continues in some countries. In Brazil, the PFOS-precursor N-ethyl perfluorooctane sulfonamide (EtFOSA) is used in Sulfluramid, a pesticide for controlling leaf-cutting ants. New data on production, environmental fate, and occurrence of Brazilian Sulfluramid are reported herein. From 2003 to 2013, Brazilian Sulfluramid manufacturing increased from 30 to 60 tonnes yr⁻¹ EtFOSA. During this time <1.3 tonnes yr⁻¹ were imported, while exports increased from approximately 0.3 to 2 tonnes yr⁻¹. From 2004 to 2015, most EtFOSA was exported to Argentina (7.2 tonnes), Colombia (2.07 tonnes), Costa Rica (1.13 tonnes), Ecuador (2.16 tonnes), and Venezuela (2.4 tonnes). Within Brazil, sales occurred primarily in the states of Minas Gerais, Sao Paulo, Mato Grosso do Sul, Espirito Santo, and Bahia. Model simulations predict EtFOSA will partition to soils, while transformation products perfluorooctane sulfonamide (FOSA) and PFOS are sufficiently mobile to leach into surface waters. In support of these predictions, up to 3400 pg L⁻¹ of FOSA and up to 1100 pg L⁻¹ of PFOS were measured in Brazilian surface water, while EtFOSA was not detected. The high FOSA/PFOS ratio observed here (up to 14:1) is unprecedented in the scientific literature to our knowledge. Depending on the extent of conversion of EtFOSA, cumulative Brazilian Sulfluramid production and import from 2004 to 2015 may contribute between 167 and 487 tonnes of PFOS/FOSA to the environment. These levels are clearly nontrivial and of concern since production is continuing unabated.

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 LA - eng
 PT - Journal Article
 DEP - 20151224
 PL - United States
 TA - Environ Sci Technol
 JT - Environmental science & technology
 JID - 0213155
 SB - IM
 EDAT- 2015/12/15 06:00
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 PHST- 2015/12/24 [aheadofprint]
 AID - 10.1021/acs.est.5b04544 [doi]
 PST - ppublish
 SO - Environ Sci Technol. 2016 Jan 19;50(2):653-9. doi: 10.1021/acs.est.5b04544. Epub 2015 Dec 24.

 PMID- 26649981
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160119
 IS - 1520-5851 (Electronic)
 IS - 0013-936X (Linking)
 VI - 50
 IP - 2
 DP - 2016 Jan 19
 TI - A New Fluorinated Surfactant Contaminant in Biota: Perfluorobutane Sulfonamide in Several Fish Species.
 PG - 669-75
 LID - 10.1021/acs.est.5b05058 [doi]
 AB - Environmental contamination and regulation of longer-chain perfluoroalkyl substances (PFASs) such as perfluorooctanesulfonate (PFOS) has given rise to the increased use of shorter-chain PFASs as alternatives in new products, although confirmation of their presence in the environment remains limited. In this study, the PFAS alternative, perfluoro-1-butane-sulfonamide (FBSA), was identified for the first time in biota in homogenate samples of fish by liquid chromatography-quadrupole time-of-flight mass spectrometry (LC-Q-ToF-MS) and quantified by ultra high performance liquid chromatography-triple quadrupole mass spectrometry (UHPLC-QQQ-MS/MS). In one flounder (*Platichthys flesus*) muscle sample from the Western Scheldt, The Netherlands, FBSA concentration was at 80.12

ng/g wet weight (w.w.) and was exceeded only by PFOS. FBSA was also detected in 32 out of 33 samples of freshwater fish collected (2009-2010) from water bodies across Canada. In lake trout (*Salvelinus namaycush*) from northern Canada (e.g., Lake Kusawa (Yukon Territory), Great Bear Lake (Northwest Territories and in the Arctic), and Lake Athabasca (northern Alberta)), the concentrations of FBSA ranged from below method detection limit (<0.01 ng/g w.w) to 0.44 ng/g w.w. and were much lower than those reported for lake trout from the more urbanized and industrialized Laurentian Great Lakes sites (3.17 +/- 1.53 ng/g w.w.). In three species of fish purchased from a supermarket in Ottawa (ON, Canada), FBSA concentrations were the lowest of all fish and ranged from < MLOD to 0.29 ng/g w.w. and 0.03 to 0.76 ng/g w.w. in muscle and liver, respectively. FBSA is a bioaccumulative contaminant in fish in Canada and possibly in The Netherlands. It is likely sourced from new alternative perfluorobutane-based products, as well as other shorter chain perfluoroalkyl-based products.

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LA - eng

PT - Journal Article

DEP - 20151228

PL - United States

TA - Environ Sci Technol

JT - Environmental science & technology

JID - 0213155

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EDAT- 2015/12/10 06:00

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AID - 10.1021/acs.est.5b05058 [doi]

PST - ppublish

SO - Environ Sci Technol. 2016 Jan 19;50(2):669-75. doi: 10.1021/acs.est.5b05058. Epub
2015 Dec 28.

PMID- 26636476
OWN - NLM
STAT- In-Data-Review
DA - 20151215
IS - 1520-5851 (Electronic)
IS - 0013-936X (Linking)
VI - 49
IP - 24
DP - 2015 Dec 15
TI - Correction to Alternative and Legacy Perfluoroalkyl Substances: Differences
between European and Chinese River/Estuary Systems.
PG - 14742-3
LID - 10.1021/acs.est.5b05591 [doi]
FAU - Heydebreck, Franziska
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FAU - Ebinghaus, Ralf
AU - Ebinghaus R
LA - eng
PT - Journal Article
DEP - 20151204
PL - United States
TA - Environ Sci Technol
JT - Environmental science & technology
JID - 0213155
SB - IM
EDAT- 2015/12/05 06:00
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CRDT- 2015/12/05 06:00
PHST- 2015/12/04 [aheadofprint]
AID - 10.1021/acs.est.5b05591 [doi]
PST - ppublish
SO - Environ Sci Technol. 2015 Dec 15;49(24):14742-3. doi: 10.1021/acs.est.5b05591.
Epub 2015 Dec 4.

PMID- 26579583
OWN - NLM
STAT- In-Data-Review
DA - 20151215
IS - 1520-5851 (Electronic)
IS - 0013-936X (Linking)
VI - 49
IP - 24
DP - 2015 Dec 15

TI - From Spill to Sequestration: The Molecular Journey of Contamination via Comprehensive Multiphase NMR.

PG - 13983-91

LID - 10.1021/acs.est.5b03251 [doi]

AB - Comprehensive multiphase NMR is a novel NMR technique that permits all components (solutions, gels, and solids) to be studied in unaltered natural samples. In this study a wide range of CMP-NMR interaction and editing-based experiments are combined to follow contaminants (pentafluorophenol (PFP) and perfluorooctanoic acid (PFOA)) from the solution state (after a spill) through the gel-state and finally into the true solid-state (sequestered) in an intact water-swollen soil. Kinetics experiments monitoring each phase illustrate PFOA rapidly transfers from solution to the solid phase while for PFP the process is slower with longer residence times in the solution and gel phase. Interaction-based experiments reveal that PFOA enters the soil via its hydrophobic tails and selectively binds to soil microbial protein. PFP sorption shows less specificity exhibiting interactions with a range of gel and solid soil components with a preference toward aromatics (mainly lignin). The results indicate that in addition to more traditional measurements such as Koc, other factors including the influence of the contaminant on the soil-water interface, specific biological interactions, soil composition (content of lignin, protein, etc.) and physical accessibility/swellability of soil organic components will likely be central to better explaining and predicting the true behavior of contaminants in soil.

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 LA - eng
 PT - Journal Article
 DEP - 20151202
 PL - United States
 TA - Environ Sci Technol
 JT - Environmental science & technology
 JID - 0213155
 SB - IM
 EDAT- 2015/11/19 06:00
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 CRDT- 2015/11/19 06:00
 PHST- 2015/12/02 [aheadofprint]
 AID - 10.1021/acs.est.5b03251 [doi]
 PST - ppublish
 SO - Environ Sci Technol. 2015 Dec 15;49(24):13983-91. doi: 10.1021/acs.est.5b03251. Epub 2015 Dec 2.

 PMID- 26560673
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151215
 IS - 1520-5851 (Electronic)
 IS - 0013-936X (Linking)
 VI - 49
 IP - 24
 DP - 2015 Dec 15
 TI - Tissue Distribution and Whole Body Burden of the Chlorinated Polyfluoroalkyl Ether Sulfonic Acid F-53B in Crucian Carp (*Carassius carassius*): Evidence for a Highly Bioaccumulative Contaminant of Emerging Concern.
 PG - 14156-65
 LID - 10.1021/acs.est.5b04299 [doi]
 AB - Following the global actions to phase out perfluorooctanesulfonic acid (PFOS) a large number of alternative per- and polyfluoroalkyl substances, with poorly defined hazard properties, are being used in increasing quantities. Here, we report on the first detection of the chlorinated polyfluoroalkyl ether sulfonic acid F-53B in biological samples and determine the tissue distribution and whole body bioaccumulation factors (BAF_{whole body}) in crucian carp (*Carassius carassius*). Analysis of fish samples from Xiaoqing River (XR) and Tangxun Lake (TL) demonstrated a similar level of F-53B contamination with median

concentrations in blood of 41.9 and 20.9 ng/g, respectively. Tissue/blood ratios showed that distribution of F-53B primarily occurs to the kidney (TL: 0.48, XR: 0.54), gonad (TL: 0.36, XR: 0.54), liver (TL: 0.38, XR: 0.53), and heart (TL: 0.47, XR: 0.47). Median Log BAFwhole body values for F-53B (XR: 4.124, TL: 4.322) exceeded regulatory bioaccumulation criterion and were significantly higher than those of PFOS in the same data sets (XR: 3.430, TL: 3.279). On the basis of its apparent omnipresence and strong bioaccumulation propensity, it is hypothesized that F-53B could explain a significant fraction of previously unidentified organofluorine in biological samples from China, and regulatory actions for this compound are encouraged.

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LA - eng

PT - Journal Article

DEP - 20151124

PL - United States

TA - Environ Sci Technol
 JT - Environmental science & technology
 JID - 0213155
 SB - IM
 EDAT- 2015/11/13 06:00
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 PHST- 2015/11/24 [aheadofprint]
 AID - 10.1021/acs.est.5b04299 [doi]
 PST - ppublish
 SO - Environ Sci Technol. 2015 Dec 15;49(24):14156-65. doi: 10.1021/acs.est.5b04299.
 Epub 2015 Nov 24.

PMID- 26526296
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151215
 IS - 1520-5851 (Electronic)
 IS - 0013-936X (Linking)
 VI - 49
 IP - 24
 DP - 2015 Dec 15
 TI - Abiotic Hydrolysis of Fluorotelomer-Based Polymers as a Source of
 Perfluorocarboxylates at the Global Scale.
 PG - 14129-35
 LID - 10.1021/acs.est.5b03686 [doi]
 AB - Fluorotelomer-based polymers (FTPs) are the main product of the fluorotelomer
 industry. For nearly 10 years, whether FTPs degrade to form perfluorooctanoate
 (PFOA) and perfluorocarboxylate (PFCA) homologues has been vigorously contested.
 Here we show that circum-neutral abiotic hydrolysis of a commercial FTP proceeds
 with half-life estimates of 55-89 years and that base-mediated hydrolysis
 overtakes neutral hydrolysis at about pH = 10, with a half-life of approximately
 0.7 years at pH approximately 12. Considered in light of the large production
 volume of FTPs and the poor efficacy of conventional treatments for recovery of
 PFCAs from waste streams, these results suggest that FTPs manufactured to date
 potentially could increase PFCAs 4- to 8-fold over current oceanic loads, largely
 depending on the integrity of disposal units to contain PFCAs upon hydrolytic
 generation from FTPs.
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 LA - eng
 PT - Journal Article

DEP - 20151124
 PL - United States
 TA - Environ Sci Technol
 JT - Environmental science & technology
 JID - 0213155
 SB - IM
 EDAT- 2015/11/04 06:00
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 CRDT- 2015/11/04 06:00
 PHST- 2015/11/24 [aheadofprint]
 AID - 10.1021/acs.est.5b03686 [doi]
 PST - ppublish
 SO - Environ Sci Technol. 2015 Dec 15;49(24):14129-35. doi: 10.1021/acs.est.5b03686.
 Epub 2015 Nov 24.

PMID- 26000882
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151215
 IS - 1520-5851 (Electronic)
 IS - 0013-936X (Linking)
 VI - 49
 IP - 24
 DP - 2015 Dec 15
 TI - World-Wide Indoor Exposure to Polyfluoroalkyl Phosphate Esters (PAPs) and other
 PFASs in Household Dust.
 PG - 14503-11
 LID - 10.1021/acs.est.5b00679 [doi]
 AB - Human exposure to perfluorooctanoic acid (PFOA) and other per- and
 polyfluoroalkyl substances (PFASs) is ongoing and in some cases increasing,
 despite efforts made to reduce emissions. The role of precursor compounds such as
 polyfluorinated phosphate esters (PAPs) has received increasing attention, but
 there are knowledge gaps regarding their occurrence and impact on human exposure.
 In this study, mono-, di-, and triPAPs, perfluorinated alkyl acids (PFAAs),
 saturated, and unsaturated fluorotelomer carboxylic acids (FTCA/FTUCAs),
 perfluoroalkane sulfonamides, and sulfonamidethanols (FOSA/FOSEs), and one
 fluorotelomer sulfonic acid (FTSA)) were compared in household dust samples from
 Canada, the Faroe Islands, Sweden, Greece, Spain, Nepal, Japan, and Australia.
 Mono-, di-, and triPAPs, including several diPAP homologues, were frequently
 detected in dust from all countries, revealing an ubiquitous spread in private
 households from diverse geographic areas, with significant differences between
 countries. The median levels of monoPAPs and diPAPs ranged from 3.7 ng/g to 1 023
 ng/g and 3.6 ng/g to 692 ng/g, respectively, with the lowest levels found in
 Nepal and the highest in Japan. The levels of PAPs exceeded those of the other
 PFAS classes. These findings reveal the importance of PAPs as a source of PFAS
 exposure worldwide.

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LA - eng

PT - Journal Article

DEP - 20150602

PL - United States

TA - Environ Sci Technol

JT - Environmental science & technology

JID - 0213155

SB - IM

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PHST- 2015/06/02 [aheadofprint]

AID - 10.1021/acs.est.5b00679 [doi]

PST - ppublish

SO - Environ Sci Technol. 2015 Dec 15;49(24):14503-11. doi: 10.1021/acs.est.5b00679. Epub 2015 Jun 2.

PMID- 26053759

OWN - NLM

STAT- In-Data-Review

DA - 20151201

IS - 1520-5851 (Electronic)

IS - 0013-936X (Linking)

VI - 49

IP - 23

DP - 2015 Dec 1

TI - In Vivo and in Vitro Isomer-Specific Biotransformation of Perfluorooctane Sulfonamide in Common Carp (*Cyprinus carpio*).

PG - 13817-24

LID - 10.1021/acs.est.5b00488 [doi]

AB - Biotransformation of PFOS-precursors (PreFOS) may contribute significantly to the level of perfluorooctanesulfonate (PFOS) in the environment. Perfluorooctane sulfonamide (PFOSA) is one of the major intermediates of higher molecular weight PreFOS. Its further degradation to PFOS could be isomer specific and thereby explain unexpected high percentages of branched (Br-) PFOS isomers observed in wildlife. In this study, isomeric degradation of PFOSA was concomitantly investigated by in vivo and in vitro tests using common carp as an animal model. In the in vivo tests branched isomers of PFOSA and PFOS were eliminated faster than the corresponding linear (n-) isomers, leading to enrichment of n-PFOSA in the fish. In contrast, Br-PFOS was enriched in the fish, suggesting that Br-PFOSA isomers were preferentially metabolized to Br-PFOS over n-PFOSA. This was confirmed by the in vitro test. The exception was 1m-PFOSA, which could be the

most difficult to be metabolized due to its alpha-branched structure, resulting in the deficiency of 1m-PFOS in the fish. The in vitro tests indicated that the metabolism mainly took place in the fish liver instead of its kidney, and it was mainly a Phase I reaction. The results may help to explain the special PFOS isomer profile observed in wildlife.

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LA - eng

PT - Journal Article

DEP - 20151120

PL - United States

TA - Environ Sci Technol

JT - Environmental science & technology

JID - 0213155

SB - IM

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AID - 10.1021/acs.est.5b00488 [doi]
PST - ppublish
SO - Environ Sci Technol. 2015 Dec 1;49(23):13817-24. doi: 10.1021/acs.est.5b00488.
Epub 2015 Nov 20.

PMID- 26724606
OWN - NLM
STAT- Publisher
DA - 20160102
LR - 20160103
IS - 1872-7077 (Electronic)
IS - 1382-6689 (Linking)
VI - 41
DP - 2015 Dec 21
TI - Hepatic miRNA profiles and thyroid hormone homeostasis in rats exposed to dietary
potassium perfluorooctanesulfonate (PFOS).
PG - 201-210
LID - S1382-6689(15)30151-4 [pii]
LID - 10.1016/j.etap.2015.12.009 [doi]
AB - Perfluorooctanesulfonate (PFOS) has been widely used in a variety of industrial
and commercial applications as a surfactant and stain repellent. PFOS causes
liver damage (including liver tumors) in experimental animals, primarily via
interaction with PPARalpha and CAR/PXR. We investigated the involvement of
microRNAs (miRNAs) in PFOS-induced hepatotoxicity, and mechanisms involved in
abnormal thyroid hormone (TH) homeostasis, in the livers of adult male rats
exposed in feed to 50mg PFOS/kg diet for 28 days. PFOS-treated rats exhibited
expected histopathological and clinical chemistry changes, and global gene
expression changes consistent with the involvement of PPARalpha and CAR/PXR.
Thirty-eight miRNAs were significantly altered. Three members of the miR-200
family were the most increased, while miR-122-5p and miR-21-5p were the most
decreased, in PFOS-treated rats. Expression of the miR-23b-3p/27b-3p/24-3p
cluster also decreased in PFOS-treated animals. Pathway analysis of miRNAs and
associated gene expression changes suggests involvement of epithelial to
mesenchymal transition (EMT), which is a primary process of tumor cell motility
and cancer metastasis. Our analysis also revealed transcripts that may mediate
PFOS-induced effects on TH homeostasis including: activation of the CAR/PXR
pathway, phase II/III enzymes, and deiodinase. These changes are consistent with
low serum TH due to enhanced metabolic clearance of TH. However, most TH hepatic
target genes were not altered in a manner consistent with reduced TH signaling,
suggesting that PFOS exposure did not induce functional hypothyroidism.
Collectively, the study suggests an important role for miRNAs in PFOS-induced
hepatotoxicity and provides insight into the effects of PFOS on TH homeostasis.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151221

TA - Environ Toxicol Pharmacol

JT - Environmental toxicology and pharmacology

JID - 9612020

OTO - NOTNLM

OT - EMT

OT - Liver

OT - Microarray

OT - PFOS

OT - miRNA

EDAT- 2016/01/03 06:00

MHDA- 2016/01/03 06:00

CRDT- 2016/01/03 06:00

PHST- 2015/08/28 [received]

PHST- 2015/11/30 [revised]

PHST- 2015/12/17 [accepted]

AID - S1382-6689(15)30151-4 [pii]

AID - 10.1016/j.etap.2015.12.009 [doi]

PST - aheadofprint

SO - Environ Toxicol Pharmacol. 2015 Dec 21;41:201-210. doi: 10.1016/j.etap.2015.12.009.

PMID- 26366629

OWN - NLM

STAT- In-Data-Review

DA - 20151127

IS - 1944-0057 (Electronic)

IS - 1944-0057 (Linking)

VI - 32

IP - 12

DP - 2015 Dec

TI - Determination of perfluoroalkylated substances (PFASs) in drinking water from the Netherlands and Greece.

PG - 2048-57

LID - 10.1080/19440049.2015.1086823 [doi]

AB - In the present study 11 perfluoroalkylated substances (PFASs) were analysed in drinking tap water samples from the Netherlands (n = 37) and from Greece (n = 43) by applying LC-MS/MS and isotope dilution. PFASs concentrations above the limit of quantification, LOQ (0.6 ng/l) were detected in 20.9% of the samples from Greece. Total PFAS concentrations ranged between <LOQ and 5.9 ng/l, with the highest concentrations noted for the three Aegean islands Mykonos, Kalymnos and Syros and for the town Tripoli in the Peloponnese. In the Dutch situation, total PFASs concentrations above the LOQ were detected in 48.6% of the samples, varying from <LOQ to 54 ng/l. The highest concentrations were detected around Amsterdam (including Schiphol airport) and more generally, PFASs were detected in the drinking water from the western part of the Netherlands. This seems attributable to the source, which is purified surface water in this area. Short-chain PFASs and especially perfluoropentanoic acid (PFPeA), perfluorohexanoic acid (PFHxA), perfluoroheptanoic acid (PFHpA), perfluorooctanoic acid (PFOA), perfluorobutane sulfonate (PFBS), and perfluorohexane sulfonate (PFHxS) were detected most frequently, whereas long-chain PFASs (C > 8) were only rarely detected. In the drinking water samples from the eastern part of the Netherlands, where drinking water is sourced from groundwater reservoirs, no PFASs were detected. This demonstrates that exposure to PFASs through drinking water in the Netherlands is dependent on the source. Additionally, five samples of bottled water from each country were analysed in the current study, with all of them originating from ground wells. In these samples, all PFASs were below the LOQ.

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LA - eng

PT - Journal Article

DEP - 20151105

PL - England

TA - Food Addit Contam Part A Chem Anal Control Expo Risk Assess

JT - Food additives & contaminants. Part A, Chemistry, analysis, control, exposure & risk assessment

JID - 101485040

SB - IM

OTO - NOTNLM

OT - Greece

OT - Netherlands

OT - PFASs

OT - bottled water

OT - drinking tap water

OT - surface water

EDAT- 2015/09/15 06:00

MHDA- 2015/09/15 06:00

CRDT- 2015/09/15 06:00

PHST- 2015/11/05 [aheadofprint]

AID - 10.1080/19440049.2015.1086823 [doi]

PST - ppublish

SO - Food Addit Contam Part A Chem Anal Control Expo Risk Assess. 2015 Dec;32(12):2048-57. doi: 10.1080/19440049.2015.1086823. Epub 2015 Nov 5.

PMID- 26748415

OWN - NLM

STAT- Publisher

DA - 20160110

LR - 20160111

IS - 1879-0267 (Electronic)
IS - 0020-1383 (Linking)
DP - 2015 Dec 2
TI - What is the optimal salvage procedure for cut-out after surgical fixation of trochanteric fractures with the PFNA or TFN?: A multicentre study.
LID - S0020-1383(15)00749-4 [pii]
LID - 10.1016/j.injury.2015.11.027 [doi]
AB - PURPOSE: To evaluate the outcome after different types of revision operations for blade 'cut-out' and 'cut-through' after fixation of trochanteric fractures with proximal femoral nail antirotation (PFNA) or a trochanter fixation nail (TFN). METHODS: Twenty hospitals participated in this multicentre study. A total of 4109 patients were retrospectively screened for cut-out or cut-through complications after nailing of trochanteric fractures using PFNA or TFN. Fifty-seven patients (28 with 'cut-through' and 29 with 'cut-out') were included in the study. In the 'cut-through' group, 16 patients underwent a blade exchange, six patients had a blade exchange with bone cement augmentation, and six received total hip arthroplasty (THA). In the 'cut-out' group, three patients had a blade exchange, one had a blade exchange with augmentation, three underwent re-nailing of the fracture with a new PFNA, one had a girdlestone procedure and 21 had THA procedures. RESULTS: In the 'cut-through' group, eight patients who had a blade exchanges (50%) and two patients with blade exchange and augmentation (33%) required further revision operations. THA was the definite treatment in all 6 cases. In the 'cut-out' group, two patients (66%) who had blade exchanges and two (66%) who underwent re-nailing required additional revision operations during the subsequent course. One patient (4%) who had total hip arthroplasty needed revision surgery for acetabular replacement. Overall, a total of 81 revision procedures were performed. CONCLUSION: Based on the data from this study, we recommend THA as the only valid salvage procedure for 'cut-out' and 'cut-through' of helical blades after fixation of trochanteric fractures with the PFNA and TFN.
CI - Copyright (c) 2015 Elsevier Ltd. All rights reserved.
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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151202

TA - Injury

JT - Injury

JID - 0226040

OTO - NOTNLM

OT - Cut-out

OT - Cut-through

OT - PFNA

OT - Revision

OT - TFN

EDAT- 2016/01/11 06:00

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PHST- 2015/07/13 [received]

PHST- 2015/11/13 [accepted]

AID - S0020-1383(15)00749-4 [pii]

AID - 10.1016/j.injury.2015.11.027 [doi]

PST - aheadofprint

SO - Injury. 2015 Dec 2. pii: S0020-1383(15)00749-4. doi:
10.1016/j.injury.2015.11.027.

PMID- 26482482

OWN - NLM

STAT- In-Data-Review

DA - 20151215

IS - 1879-0267 (Electronic)

IS - 0020-1383 (Linking)

VI - 46

IP - 12

DP - 2015 Dec

TI - Comparison of the reconstruction trochanteric antigrade nail (TAN) with the proximal femoral nail antirotation (PFNA) in the management of reverse oblique intertrochanteric hip fractures.

PG - 2389-93

LID - 10.1016/j.injury.2015.09.038 [doi]

LID - S0020-1383(15)00576-8 [pii]

AB - Reverse oblique intertrochanteric fractures have unique mechanical characteristics and are often treated with intramedullary implants. We compared the outcomes of the reconstruction trochanteric antegrade nail (TAN) with the proximal femoral nail antirotation (PFNA). Between July 2008 and February 2014, we reviewed all patients with reverse oblique intertrochanteric fractures treated at our hospital. Patients with pathological fractures and those who were treated with other than TAN and PFNA nailing systems were excluded. Preoperative assessment included the Abbreviated mental test score (AMT), the ASA grade, pre-injury mobility and place of residence. Postoperative outcome measures included the type of implant used, time to fracture union, failures of fixation and revision surgeries. Fifty-eight patients were included and divided into two groups based on the treatment: 22 patients treated with TAN and 36 patients treated with PFNA systems. The two groups were well matched with regards to demographics and fracture type. The overall union rate was similar in both groups but the time to union was shorter in the TAN group. There were 8 implant failures in the PFNA (22.2%) group compare to none in the TAN group. Implant failure was associated with the severity of fracture (AO 31.A3.3) but was not related to fracture malreduction or screw position (Tip-apex-distance). Our study suggests that the use of reconstruction system with two screws such as TAN may be more suitable implant for reverse oblique intertrochanteric hip fractures.

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 LA - eng
 PT - Journal Article
 DEP - 20151013
 PL - Netherlands
 TA - Injury
 JT - Injury
 JID - 0226040
 SB - IM
 OTO - NOTNLM
 OT - Elderly patients
 OT - Intertrochanteric hip fractures
 OT - Proximal Femoral Nail Antirotation (PFNA)
 OT - Reverse oblique
 OT - Trochanteric Antigrade Nail (TAN)
 EDAT- 2015/10/21 06:00
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 CRDT- 2015/10/21 06:00
 PHST- 2015/07/20 [received]
 PHST- 2015/09/13 [revised]
 PHST- 2015/09/29 [accepted]
 PHST- 2015/10/13 [aheadofprint]
 AID - S0020-1383(15)00576-8 [pii]
 AID - 10.1016/j.injury.2015.09.038 [doi]
 PST - ppublish
 SO - Injury. 2015 Dec;46(12):2389-93. doi: 10.1016/j.injury.2015.09.038. Epub 2015 Oct
 13.

 PMID- 26690195
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151222
 LR - 20160107
 IS - 1660-4601 (Electronic)
 IS - 1660-4601 (Linking)
 VI - 12
 IP - 12
 DP - 2015
 TI - Investigation of the Effects of Perfluorooctanoic Acid (PFOA) and Perfluorooctane
 Sulfonate (PFOS) on Apoptosis and Cell Cycle in a Zebrafish (Danio rerio) Liver
 Cell Line.
 PG - 15673-82
 LID - 10.3390/ijerph121215012 [doi]
 AB - This study aimed to explore the effects of perfluorooctanoic acid (PFOA) and
 perfluorooctane sulfonate (PFOS) on apoptosis and cell cycle in a zebrafish

(*Danio rerio*) liver cell line (ZFL). Treatment groups included a control group, PFOA-IC50, PFOA-IC80, PFOS-IC50 and PFOS-IC80 groups. IC50 and IC80 concentrations were identified by cellular modeling and MTT assays. mRNA levels of p53, Bcl-2, Bax, Caspase-3 and NF-kappaB p65 were detected by qPCR. Cell apoptosis and cell cycle were detected by flow cytometry and the protein levels of p53, Bcl-2, Bax, Caspase-3 and NF-kappaB p65 were determined by western blotting. Both PFOA and PFOS inhibited the growth of zebrafish liver cells, and the inhibition rate of PFOS was higher than that of PFOA. Bcl-2 expression levels in the four groups were significantly higher than the control group and Bcl-2 increased significantly in the PFOA-IC80 group. However, the expression levels of Bax in the four treatment groups were higher than the control group. The percentage of cell apoptosis increased significantly with the treatment of PFOA and PFOS ($p < 0.05$). Cell cycle and cell proliferation were blocked in both the PFOA-IC80 and PFOS-IC80 groups, indicating that PFOA-IC80 and PFOS-IC50 enhanced apoptosis in ZFL cells.

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LA - eng

PT - Journal Article

DEP - 20151209

PL - Switzerland

TA - Int J Environ Res Public Health

JT - International journal of environmental research and public health

JID - 101238455

SB - IM

PMC - PMC4690948

OID - NLM: PMC4690948
 OTO - NOTNLM
 OT - apoptosis
 OT - perfluorooctane sulfonate (PFOS)
 OT - perfluorooctanoic acid (PFOA)
 OT - zebrafish liver cells (ZFL)
 EDAT- 2015/12/23 06:00
 MHDA- 2015/12/23 06:00
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 PHST- 2015/10/19 [revised]
 PHST- 2015/11/26 [accepted]
 AID - ijerph121215012 [pii]
 AID - 10.3390/ijerph121215012 [doi]
 PST - epubli
 SO - Int J Environ Res Public Health. 2015 Dec 9;12(12):15673-82. doi:
 10.3390/ijerph121215012.

 PMID- 26459765
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151120
 IS - 1791-244X (Electronic)
 IS - 1107-3756 (Linking)
 VI - 36
 IP - 6
 DP - 2015 Dec
 TI - Perfluoroheptanoic acid affects amphibian embryogenesis by inducing the
 phosphorylation of ERK and JNK.
 PG - 1693-700
 LID - 10.3892/ijmm.2015.2370 [doi]
 AB - Perfluoroalkyl compounds (PFCs) are globally distributed synthetic compounds that
 are known to adversely affect human health. Developmental toxicity assessment of
 PFCs is important to facilitate the evaluation of their environmental impact. In
 the present study, we assessed the developmental toxicity and teratogenicity of
 PFCs with different numbers of carbon atoms on *Xenopus* embryogenesis. An initial
 frog embryo teratogenicity assay-*Xenopus* (FETAX) assay was performed that
 identified perfluorohexanoic (PFHxA) and perfluoroheptanoic (PFHpA) acids as
 potential teratogens and developmental toxicants. The mechanism underlying this
 teratogenicity was also investigated by measuring the expression of
 tissue-specific biomarkers such as phosphotyrosine-binding protein, xPTB (liver);
 NKX2.5 (heart); and Cyl18 (intestine). Wholemount in situ hybridization, reverse
 transcriptase-polymerase chain reaction (RT-PCR), and histologic analyses detected
 severe defects in the liver and heart following exposure to PFHxA or PFHpA. In
 addition, immunoblotting revealed that PFHpA significantly increased the
 phosphorylation of extracellular signal-regulated kinase (ERK) and c-Jun
 N-terminal kinase (JNK), while PFHxA slightly increased these, as compared with
 the control. These results suggest that PFHxA and PFHpA are developmental

toxicants and teratogens, with PFHpA producing more severe effects on liver and heart development through the induction of ERK and JNK phosphorylation.

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LA - eng

PT - Journal Article

DEP - 20151012

PL - Greece

TA - Int J Mol Med

JT - International journal of molecular medicine

JID - 9810955

SB - IM

EDAT- 2015/10/16 06:00

MHDA- 2015/10/16 06:00

CRDT- 2015/10/14 06:00

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PHST- 2015/10/12 [aheadofprint]

AID - 10.3892/ijmm.2015.2370 [doi]

PST - ppublish

SO - Int J Mol Med. 2015 Dec;36(6):1693-700. doi: 10.3892/ijmm.2015.2370. Epub 2015
Oct 12.

PMID- 26684745

OWN - NLM

STAT- In-Data-Review

DA - 20151230

IS - 1520-5118 (Electronic)

IS - 0021-8561 (Linking)

VI - 63

IP - 51

DP - 2015 Dec 30

TI - Perfluorooctane Sulfonate Plasma Half-Life Determination and Long-Term Tissue
Distribution in Beef Cattle (Bos taurus).

PG - 10988-94

LID - 10.1021/acs.jafc.5b04565 [doi]

AB - Perfluorooctane sulfonate (PFOS) is used in consumer products as a surfactant and
is found in industrial and consumer waste, which ends up in wastewater treatment
plants (WWTPs). PFOS does not breakdown during WWTP processes and accumulates in
the biosolids. Common practices include application of biosolids to pastures and
croplands used for feed, and as a result, animals such as beef cattle are exposed
to PFOS. To determine plasma and tissue depletion kinetics in cattle, 2 steers
and 4 heifers were dosed with PFOS at 0.098 mg/kg body weight and 9.1 mg/kg,
respectively. Plasma depletion half-lives for steers and heifers were 120 +/- 4.1
and 106 +/- 23.1 days, respectively. Specific tissue depletion half-lives ranged

from 36 to 385 days for intraperitoneal fat, back fat, muscle, liver, bone, and kidney. These data indicate that PFOS in beef cattle has a sufficiently long depletion half-life to permit accumulation in edible tissues.

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LA - eng

PT - Journal Article

DEP - 20151218

PL - United States

TA - J Agric Food Chem

JT - Journal of agricultural and food chemistry

JID - 0374755

SB - IM

OTO - NOTNLM

OT - PFOS

OT - beef cattle

OT - food safety

OT - half-life

OT - perfluorooctane sulfonate

OT - plasma

OT - residue

EDAT- 2015/12/20 06:00

MHDA- 2015/12/20 06:00

CRDT- 2015/12/20 06:00

PHST- 2015/12/18 [aheadofprint]

AID - 10.1021/acs.jafc.5b04565 [doi]

PST - ppublish

SO - J Agric Food Chem. 2015 Dec 30;63(51):10988-94. doi: 10.1021/acs.jafc.5b04565.
Epub 2015 Dec 18.

PMID- 26674217

OWN - NLM

STAT- In-Data-Review

DA - 20151230

IS - 1520-5126 (Electronic)

IS - 0002-7863 (Linking)

VI - 137

IP - 51

DP - 2015 Dec 30

TI - Perfluoroalkyl Cobalt(III) Fluoride and Bis(perfluoroalkyl) Complexes: Catalytic Fluorination and Selective Difluorocarbene Formation.

PG - 16064-73

LID - 10.1021/jacs.5b12003 [doi]

AB - Four perfluoroalkyl cobalt(III) fluoride complexes have been synthesized and characterized by elemental analysis, multinuclear NMR spectroscopy, X-ray crystallography, and powder X-ray diffraction. The remarkable cobalt fluoride (¹⁹F NMR chemical shifts (-716 to -759 ppm) were studied computationally, and the contributing paramagnetic and diamagnetic factors were extracted. Additionally, the complexes were shown to be active in the catalytic fluorination of p-toluoyl chloride. Furthermore, two examples of cobalt(III) bis(perfluoroalkyl) complexes were synthesized and their reactivity studied. Interestingly, abstraction of a fluoride ion from these complexes led to selective formation of cobalt difluorocarbene complexes derived from the trifluoromethyl ligand. These electrophilic difluorocarbenes were shown to undergo insertion into the remaining perfluoroalkyl fragment, demonstrating the elongation of a perfluoroalkyl chain arising from a difluorocarbene insertion on a cobalt metal center. The reactions of both the fluoride and bis(perfluoroalkyl) complexes provide insight into the potential catalytic applications of these model systems to form small fluorinated molecules as well as fluoropolymers.

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LA - eng

PT - Journal Article

DEP - 20151216

PL - United States

TA - J Am Chem Soc

JT - Journal of the American Chemical Society

JID - 7503056

SB - IM

EDAT- 2015/12/18 06:00

MHDA- 2015/12/18 06:00

CRDT- 2015/12/18 06:00

PHST- 2015/12/16 [aheadofprint]

AID - 10.1021/jacs.5b12003 [doi]

PST - ppublish

SO - J Am Chem Soc. 2015 Dec 30;137(51):16064-73. doi: 10.1021/jacs.5b12003. Epub 2015
Dec 16.

PMID- 25677194

OWN - NLM

STAT- In-Process

DA - 20151021

IS - 1099-1263 (Electronic)

IS - 0260-437X (Linking)

VI - 35

IP - 12

DP - 2015 Dec

TI - Involvement of mitogen-activated protein kinase and NF-kappaB signaling pathways in perfluorooctane sulfonic acid-induced inflammatory reaction in BV2 microglial cells.

PG - 1539-49

LID - 10.1002/jat.3119 [doi]

AB - Microglial activation is closely related to the pathogenesis of neurodegenerative diseases by producing proinflammatory cytokines. Perfluorooctane sulfonic acid (PFOS), known as an emerging persistent organic pollutant, is reported to disturb human immune homeostasis; however, whether it affects cytokine production or the immune response in the central nervous system remains unclear. The present study was aimed to explore whether PFOS contributed to inflammatory action and to investigate the corresponding mechanisms in BV2 microglia. PFOS-mediated morphologic changes, cytokine responses and signaling events were examined by light microscopy, real-time polymerase chain reaction, enzyme-linked immunosorbent assay and Western blot assays. Our results indicated that PFOS increased BV2 cells activation and simultaneously increased tumor necrosis factor alpha and interleukin-6 expression. In addition, the c-Jun N-terminal protein kinase inhibitor (SP600125), as well as ERK1/2 blocker (PD98059), transcriptionally at least, displayed anti-inflammatory properties on PFOS-elicited cytokine responses. Moreover, the inflammatory transcription factor NF-kappaB was specifically activated by PFOS as well. These results, taken together, suggested that PFOS exerts its functional effects on the response of microglial cell activation via, in part, the c-Jun N-terminal protein kinase, ERK and NF-kappaB signaling pathways with its subsequent influence on proinflammatory action.

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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

DEP - 20150212

PL - England

TA - J Appl Toxicol

JT - Journal of applied toxicology : JAT

JID - 8109495

SB - IM

OTO - NOTNLM

OT - MAPK

OT - NF-kappaB

OT - PFOS

OT - immunomodulatory cytokines

OT - microglia

EDAT- 2015/02/14 06:00

MHDA- 2015/02/14 06:00

CRDT- 2015/02/14 06:00

PHST- 2014/09/10 [received]

PHST- 2014/12/15 [revised]

PHST- 2014/12/15 [accepted]

PHST- 2015/02/12 [aheadofprint]

AID - 10.1002/jat.3119 [doi]

PST - ppublish

SO - J Appl Toxicol. 2015 Dec;35(12):1539-49. doi: 10.1002/jat.3119. Epub 2015 Feb 12.

PMID- 26364075

OWN - NLM

STAT- PubMed-not-MEDLINE

DA - 20151003

DCOM- 20151228

IS - 1095-7103 (Electronic)

IS - 0021-9797 (Linking)

VI - 460

DP - 2015 Dec 15

TI - Semifluorinated thiols in Langmuir monolayers - a study by nonlinear and linear vibrational spectroscopies.

PG - 290-302

LID - 10.1016/j.jcis.2015.08.069 [doi]

LID - S0021-9797(15)30164-8 [pii]

AB - A series of semifluorinated thiols of the general formula $C_mF_{2m+1}C_nH_{2n}SH$ (abbr. F_mH_nSH) have been synthesized and characterized in Langmuir monolayers with surface pressure-area isotherms, complemented with polarization-modulated reflection absorption spectroscopy (PM-IRRAS) and sum-frequency generation (SFG) techniques. A comparative analysis was performed for compounds having the same length of fluorinated segment (F10) and variable length of the hydrogenated part (H6, H10, H12), and having identical hydrogenated segment (H12) connected to a fluorinated moiety of different lengths (F6, F8, F10). For the sake of comparison, an alkanethiol (H18SH) was also examined, and F10H10COOH and F10H10OH molecules were used for helping the assignment of SFG spectra of CH stretches. SFG was applied to investigate the hydrocarbon chain and the terminal CF₃ group, while PM-IRRAS was used to probe CF₂ groups. The number of gauche defects in the hydrocarbon chain increased with the increasing length of the molecule, either by elongation of the hydrogenated or perfluorinated part. SFG measurements recorded at three polarization combinations (ppp, ssp, sps) enabled us to estimate the tilt angle of the terminal CF₃ group in semifluorinated thiol molecules as ranging from 35 degrees to 45 degrees, which is consistent with nearly vertical fluorinated segments. Upon increasing the surface pressure, the fluorinated segment gets slightly more upright, but the hydrocarbon chain tilt increases while keeping the same average number of gauche defects. The extent of disorder in the hydrogenated segment may be controlled by varying the size of the fluorinated segment, and this could be exploited for designing functionalized surfaces with insertion of other molecules in the defect region.

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 LA - eng
 PT - Journal Article
 DEP - 20150829
 PL - United States
 TA - J Colloid Interface Sci
 JT - Journal of colloid and interface science
 JID - 0043125
 OTO - NOTNLM
 OT - Air/water interface
 OT - Alkanethiols
 OT - Langmuir monolayers
 OT - Nonlinear spectroscopy
 OT - Polarization-modulated reflection absorption spectroscopy
 OT - Semifluorinated alkanes
 OT - Sum-frequency generation spectroscopy
 OT - Vibrational spectroscopy
 EDAT- 2015/09/14 06:00
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 PHST- 2015/07/16 [received]
 PHST- 2015/08/27 [revised]
 PHST- 2015/08/29 [accepted]
 PHST- 2015/08/29 [aheadofprint]
 AID - S0021-9797(15)30164-8 [pii]
 AID - 10.1016/j.jcis.2015.08.069 [doi]
 PST - ppublish
 SO - J Colloid Interface Sci. 2015 Dec 15;460:290-302. doi:
 10.1016/j.jcis.2015.08.069. Epub 2015 Aug 29.

 PMID- 26686481
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160109
 IS - 1873-3336 (Electronic)
 IS - 0304-3894 (Linking)
 VI - 305
 DP - 2016 Mar 15
 TI - Toxicity and bioaccumulation of copper in Limnodrilus hoffmeisteri under
 different pH values: Impacts of perfluorooctane sulfonate.
 PG - 219-28
 LID - 10.1016/j.jhazmat.2015.11.048 [doi]

LID - S0304-3894(15)30249-1 [pii]

AB - Aquatic oligochaete *Limnodrilus hoffmeisteri* (*L. hoffmeisteri*) has been commonly used as a lethal and/or sub-lethal toxicological model organism in ecological risk assessments in contaminated water environments. In this study, experiments were conducted to investigate the potential toxic effects of copper (Cu(II)) with or without perfluorooctane sulfonate (PFOS) under different pH values (6.0, 7.0 and 8.0) on LC50, bioaccumulation, and oxidative stress biomarkers in *L. hoffmeisteri* after 3 and 7 days. The LC50 values of Cu(II) decreased with the increasing pH and the addition of PFOS. After each exposure, increasing bioaccumulation of Cu(II) in *L. hoffmeisteri* was observed in the combined exposure treatments, whereas the bioaccumulation of PFOS decreased. Moreover, the activity of superoxide dismutase, the level of glutathione, and the content of malondialdehyde were significantly altered after these exposures, possibly indicating that the bioaccumulation of Cu(II) and PFOS caused adverse effects on antioxidant defenses of *L. hoffmeisteri*. The integrated biomarker response index, indicates that the combined effect was proposed as synergism, which is coincided with the results of toxic unit. Moreover, this work showed that aquatic environment may become more livable when water conditions changed from acidic to near-neutral or alkaline.

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LA - eng

PT - Journal Article

DEP - 20151202

PL - Netherlands

TA - J Hazard Mater

JT - Journal of hazardous materials

JID - 9422688

SB - IM

OTO - NOTNLM

OT - Bioaccumulation

OT - Copper

OT - Different pH values

OT - *Limnodrilus hoffmeisteri*

OT - Oxidative stress

OT - Perfluorooctane sulfonate

EDAT- 2015/12/22 06:00

MHDA- 2015/12/22 06:00

CRDT- 2015/12/22 06:00

PHST- 2015/07/29 [received]

PHST- 2015/11/04 [revised]

PHST- 2015/11/24 [accepted]

PHST- 2015/12/02 [aheadofprint]

AID - S0304-3894(15)30249-1 [pii]

AID - 10.1016/j.jhazmat.2015.11.048 [doi]

PST - ppublish

SO - J Hazard Mater. 2016 Mar 15;305:219-28. doi: 10.1016/j.jhazmat.2015.11.048. Epub 2015 Dec 2.

PMID- 26282221

OWN - NLM

STAT- In-Data-Review

DA - 20151123

IS - 1873-3336 (Electronic)

IS - 0304-3894 (Linking)

VI - 300

DP - 2015 Dec 30

TI - Effect of sound frequency and initial concentration on the sonochemical degradation of perfluorooctane sulfonate (PFOS).

PG - 662-9

LID - 10.1016/j.jhazmat.2015.07.077 [doi]

LID - S0304-3894(15)00614-7 [pii]

AB - Perfluorooctanesulfonic acid (PFOS) is a perfluorinated compound (PFC) highly

resistant to conventional advance oxidation processes, which was widely used in industrial activities due to its surfactant nature, oleophobic-hydrophobic properties, and chemical inertness. Sonochemical treatment has been suggested as an effective approach to treat aqueous solutions containing minimal levels of PFCs. This study investigates PFOS sonochemical degradation and its dependency on the initial concentration (10-460µM), and the applied sound frequency (25 and 500kHz, and 1MHz). PFOS was degraded by sonochemical treatment at concentrations as high as 460µM, as demonstrated by fluoride release and total organic content data. PFOS degradation rate was higher at megasonic frequencies (1MHz) compared to ultrasonic frequencies (25-500kHz). PFOS degradation was controlled by saturation kinetics as indicated by an increase in PFOS degradation rate with increasing PFOS concentration until a maximum, after which the degradation rate was independent of the concentration. The saturation conditions were dependent on the sound frequency, and they were reached at a lower concentration under 1MHz (100µM) compared to the 500kHz frequency (>460µM). Overall, the results of this study demonstrate that high PFOS concentration can be effectively sonochemically treated using megasonic frequencies.

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LA - eng

PT - Journal Article

DEP - 20150803

PL - Netherlands

TA - J Hazard Mater

JT - Journal of hazardous materials

JID - 9422688

SB - IM

OTO - NOTNLM

OT - Kinetics

OT - Megasonic

OT - PFOS

OT - Perfluorocarbons
 OT - Sonochemistry
 OT - Sonolysis
 OT - Ultrasonic
 EDAT- 2015/08/19 06:00
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 PHST- 2015/08/03 [aheadofprint]
 AID - S0304-3894(15)00614-7 [pii]
 AID - 10.1016/j.jhazmat.2015.07.077 [doi]
 PST - ppublish
 SO - J Hazard Mater. 2015 Dec 30;300:662-9. doi: 10.1016/j.jhazmat.2015.07.077. Epub 2015 Aug 3.

 PMID- 26280369
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151217
 IS - 1873-3336 (Electronic)
 IS - 0304-3894 (Linking)
 VI - 299
 DP - 2015 Dec 15
 TI - Occurrence, fluxes and sources of perfluoroalkyl substances with isomer analysis in the snow of northern China.
 PG - 639-46
 LID - 10.1016/j.jhazmat.2015.07.074 [doi]
 LID - S0304-3894(15)00611-1 [pii]
 AB - In this study, perfluoroalkyl substances (PFASs) and the isomers of perfluorooctanoate (PFOA) and perfluorooctanesulfonate (PFOS) were analyzed in fresh snow samples collected from 19 cities in northern China, 2013. The levels of total PFASs in the snow samples were 33.5-229ng/L, suggesting heavy atmospheric pollution of PFASs in northern China. PFOA (9.08-107ng/L), PFOS (3.52-54.3ng/L), perfluoroheptanoate (PFHpA) (3.66-44.8ng/L), and perfluorohexanoate (PFHxA) (3.21-23.6ng/L) were predominant with a summed contribution of 82% to the total PFASs. The particulate matters (PMs) associated PFASs contributed 21.5-56.2% to the total PFASs in the snow, suggesting PMs are vital for the transport and deposition of airborne PFASs. Partitioning of PFASs between PM and dissolved phases was dependent on the carbon chain length and end functional groups. Isomer profiles of PFOA and PFOS in the snow were in agreement with the signature of the historical 3M electrochemical fluorination (ECF) products, suggesting that the ECF products were still produced and used in China. Further source analysis showed that the airborne PFASs in urban area were mainly due to direct release rather than degradation of their precursors.
 CI - Copyright (c) 2015 Elsevier B.V. All rights reserved.
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LA - eng
PT - Journal Article
DEP - 20150731
PL - Netherlands
TA - J Hazard Mater
JT - Journal of hazardous materials
JID - 9422688
SB - IM
OTO - NOTNLM
OT - Isomers
OT - PFOA
OT - PFOS
OT - Snow
OT - Sources
EDAT- 2015/08/19 06:00
MHDA- 2015/08/19 06:00
CRDT- 2015/08/18 06:00
PHST- 2015/06/07 [received]
PHST- 2015/07/26 [revised]
PHST- 2015/07/29 [accepted]
PHST- 2015/07/31 [aheadofprint]
AID - S0304-3894(15)00611-1 [pii]
AID - 10.1016/j.jhazmat.2015.07.074 [doi]
PST - ppublish
SO - J Hazard Mater. 2015 Dec 15;299:639-46. doi: 10.1016/j.jhazmat.2015.07.074. Epub 2015 Jul 31.

PMID- 26183235
OWN - NLM
STAT- In-Data-Review
DA - 20151217

IS - 1873-3336 (Electronic)

IS - 0304-3894 (Linking)

VI - 299

DP - 2015 Dec 15

TI - Highly efficient electrochemical degradation of perfluorooctanoic acid (PFOA) by F-doped Ti/SnO₂ electrode.

PG - 417-24

LID - 10.1016/j.jhazmat.2015.06.033 [doi]

LID - S0304-3894(15)00489-6 [pii]

AB - The novel F-doped Ti/SnO₂ electrode prepared by SnF₄ as the single-source precursor was used for electrochemical degradation of aqueous perfluorooctanoic acid (PFOA). Higher oxidation reactivity and significantly longer service life were achieved for Ti/SnO₂-F electrode than Ti/SnO₂-X (X=Cl, Br, I, or Sb) electrode, which could decomposed over 99% of PFOA (50mL of 100mgL⁻¹) within 30-min electrolysis. The property of Ti/SnO₂-F electrode and its electrooxidation mechanism were investigated by XRD, SEM-EDX, EIS, LSV, and interfacial resistance measurements. We propose that the similar ionic radii of F and O as well as strong electronegativity of F caused its electrochemical stability with high oxygen evolution potential (OEP) and smooth surface to generate weakly adsorbed OH. The preparation conditions of electrode were also optimized including F doping amount, calcination temperature, and dip coating times, which revealed the formation process of electrode. Additionally, the major mineralization product, F⁻, and low concentration of shorter chain perfluorocarboxylic acids (PFCAs) were detected in solution. So the reaction pathway of PFOA electrooxidation was proposed by intermediate analysis. These results demonstrate that Ti/SnO₂-F electrode is promising for highly efficient treatment of PFOA in wastewater.

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LA - eng

PT - Journal Article

DEP - 20150623

PL - Netherlands

TA - J Hazard Mater

JT - Journal of hazardous materials

JID - 9422688

SB - IM

OTO - NOTNLM

OT - Electrochemical degradation

OT - F doping

OT - PFOA

OT - Ti/SnO(2) electrode

EDAT- 2015/07/18 06:00

MHDA- 2015/07/18 06:00

CRDT- 2015/07/18 06:00

PHST- 2015/04/30 [received]

PHST- 2015/05/22 [revised]

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PHST- 2015/06/23 [aheadofprint]

AID - S0304-3894(15)00489-6 [pii]

AID - 10.1016/j.jhazmat.2015.06.033 [doi]

PST - ppublish

SO - J Hazard Mater. 2015 Dec 15;299:417-24. doi: 10.1016/j.jhazmat.2015.06.033. Epub 2015 Jun 23.

PMID- 26143199

OWN - NLM

STAT- In-Data-Review

DA - 20151217

IS - 1873-3336 (Electronic)

IS - 0304-3894 (Linking)

VI - 299

DP - 2015 Dec 15

TI - Proteomic analysis of cell proliferation in a human hepatic cell line (HL-7702) induced by perfluorooctane sulfonate using iTRAQ.

PG - 361-70

LID - 10.1016/j.jhazmat.2015.06.031 [doi]

LID - S0304-3894(15)00487-2 [pii]

AB - Perfluorooctane sulfonate (PFOS) is a commonly used and widely distributed perfluorinated compound proven to cause adverse health outcomes. However, how PFOS affects liver cell proliferation is not well understood. In this experiment, we exposed a human liver cell line (HL-7702) to 50µM PFOS for 48h and 96h. We identified 52 differentially expressed proteins using a quantitative proteomic approach. Among them, 27 were associated with cell proliferation, including hepatoma-derived growth factor (Hdgf) and proliferation biomarkers Mkl67 (Ki67) and Top2alpha. Results from MTT, cell counting, and cell cycle analysis showed low-dose PFOS (<200µM) stimulated HL-7702 cell viability at 48h and 96h, reduced the G0/G1 percentage, and increased the S+G2/M percentage. Moreover, levels of Cyclin D1, Cyclin E2, Cyclin A2, Cyclin B1 and their partner Cdk5 were elevated, and the expression of regulating proteins like c-Myc, p53, p21 waf/cip1 and Myt1, as well as the phosphorylation levels of p-Wee1(S642), p-Chk1(S345) and p-Chk2(T68), were disturbed. We hypothesized that low-dose PFOS stimulated HL-7702 proliferation by driving cells into G1 through elevating cyclins/cdks expression, and by promoting cell cycle progression through altering other regulating proteins. This research will shed light on the mechanisms behind PFOS-mediated human hepatotoxicity.

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LA - eng

PT - Journal Article

DEP - 20150623

PL - Netherlands

TA - J Hazard Mater
 JT - Journal of hazardous materials
 JID - 9422688
 SB - IM
 OTO - NOTNLM
 OT - Cell cycle
 OT - Cell proliferation
 OT - Cyclins
 OT - PFOS
 OT - iTRAQ
 EDAT- 2015/07/06 06:00
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 PHST- 2015/06/23 [aheadofprint]
 AID - S0304-3894(15)00487-2 [pii]
 AID - 10.1016/j.jhazmat.2015.06.031 [doi]
 PST - ppublish
 SO - J Hazard Mater. 2015 Dec 15;299:361-70. doi: 10.1016/j.jhazmat.2015.06.031. Epub 2015 Jun 23.

 PMID- 26684582
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151228
 IS - 1873-3344 (Electronic)
 IS - 0162-0134 (Linking)
 VI - 155
 DP - 2016 Feb
 TI - Synthesis of platinum complexes with
 2-(5-perfluoroalkyl-1,2,4-oxadiazol-3yl)-pyridine and
 2-(3-perfluoroalkyl-1-methyl-1,2,4-triazole-5yl)-pyridine ligands and their in
 vitro antitumor activity.
 PG - 92-100
 LID - 10.1016/j.jinorgbio.2015.11.020 [doi]
 LID - S0162-0134(15)30122-7 [pii]
 AB - Five new mononuclear Pt(II) complexes with
 5-perfluoroalkyl-1,2,4-oxadiazolyl-pyridine and
 3-perfluoroalkyl-1,2,4-triazolyl-pyridine ligands are reported. The ligands
 2-(5-perfluoroheptyl-1,2,4-oxadiazole-3yl)-pyridine (pfhop),
 2-(5-perfluoropropyl)-1,2,4-oxadiazole-3yl)-pyridine (pfpop),
 2-(3-perfluoroheptyl-1-methyl-1,2,4-triazole-5yl)-pyridine (pfhtp),
 2-(3-perfluoropropyl-1-methyl-1,2,4-triazole-5yl)-pyridine (pfptp) and their
 complexes [PtCl2(pfhop)2].1.5 DMSO (2a), [PtCl2(pfpop)2].1.5 DMSO (3a),
 [PtCl2(pfhtp)2].1.5 DMSO (4a), PtCl2(pfhtp) (4b), [PtCl2(pfptp)2].1.5 DMSO (5a)
 have been synthesized and structurally characterized. The complexes 2a, 3a, 4a

and 5a have the same chemical environment of Pt(II) where PtCl₂ moieties coordinate two molecules of ligand via N1 atom of pyridine in the case of pfhop and pfpop, and N2 atom of 1,2,4-triazole in the case of pfhtp and pfptp. For 4b, pfhtp behaves as bidentate ligand, coordinating Pt(II) ion via N4 atom of triazole and N1 atom of pyridine. All complexes have been tested in vitro by 3-(4,5-dimethyl-2-thiazolyl)bromide-2,5-diphenyl-2H-tetrazolium (MTT) test on four tumor cell lines MCF-7 (human breast cancer), HepG2 (human hepatocellular carcinoma), HCT116 (human colorectal carcinoma). Compounds 2a and 4b showed a dose-dependent anti-proliferative effect against the three tumor cell lines whereas did not affect viability of intestinal normal-like differentiated Caco-2 cells. The cell death of HepG2, MCF-7 and HCT116 induced by the compounds, was considered to be apoptotic by measuring the exposure of phosphatidylserine to the outer membrane and observing the typical apoptotic morphological change by acridine orange (AO)/ethidium bromide (EB) staining.

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LA - eng
PT - Journal Article
DEP - 20151201
PL - United States
TA - J Inorg Biochem
JT - Journal of inorganic biochemistry
JID - 7905788
SB - IM
OTO - NOTNLM
OT - Antitumor activity
OT - Mononuclear platinum complexes
OT - Perfluoroalkyl heterocyclic ligands
EDAT- 2015/12/20 06:00
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AID - S0162-0134(15)30122-7 [pii]
AID - 10.1016/j.jinorgbio.2015.11.020 [doi]
PST - ppublish
SO - J Inorg Biochem. 2016 Feb;155:92-100. doi: 10.1016/j.jinorgbio.2015.11.020. Epub
2015 Dec 1.

PMID- 26580021
OWN - NLM
STAT- In-Data-Review
DA - 20151218
IS - 1520-6904 (Electronic)
IS - 0022-3263 (Linking)
VI - 80
IP - 24
DP - 2015 Dec 18
TI - Synthesis of Perfluorinated Isoquinolinediones through Visible-Light-Induced
Cyclization of Alkenes.
PG - 12599-605
LID - 10.1021/acs.joc.5b01803 [doi]
AB - A novel visible-light-induced carboperfluoroalkylation of alkenes using
perfluoroalkyl iodides and bromides as Rf sources, leading to
isoquinoline-1,3-diones, was developed. This method offers rapid entry to
perfluorinated isoquinoline-1,3(2H,4H)-diones from N-alkyl-N-methacryloyl
benzamides under mild reaction conditions, allowing for the incorporation of a
wide variety of perfluorinated groups such as CF3, C3F7, C4F9, C6F13, C8F17,
C10F21, and CF2CO2Et.
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LA - eng
PT - Journal Article
DEP - 20151201
PL - United States
TA - J Org Chem
JT - The Journal of organic chemistry
JID - 2985193R
SB - IM
EDAT- 2015/11/19 06:00
MHDA- 2015/11/19 06:00
CRDT- 2015/11/19 06:00

PHST- 2015/12/01 [aheadofprint]
AID - 10.1021/acs.joc.5b01803 [doi]
PST - ppublish
SO - J Org Chem. 2015 Dec 18;80(24):12599-605. doi: 10.1021/acs.joc.5b01803. Epub 2015 Dec 1.

PMID- 26550962

OWN - NLM

STAT- In-Data-Review

DA - 20151218

IS - 1520-6904 (Electronic)

IS - 0022-3263 (Linking)

VI - 80

IP - 24

DP - 2015 Dec 18

TI - Radical Reactions of Alkyl 2-Bromo-2,2-difluoroacetates with Vinyl Ethers:
"Omitted" Examples and Application for the Synthesis of 3,3-Difluoro-GABA.

PG - 12258-64

LID - 10.1021/acs.joc.5b02171 [doi]

AB - Addition reactions of perfluoroalkyl radicals to ordinary or polyfluorinated alkenes have been frequently used to synthesize perfluoroalkylated organic compounds. Here ethyl/methyl 2-bromo-2,2-difluoroacetate, diethyl (bromodifluoromethyl)phosphonate, [(bromodifluoromethyl)sulfonyl]benzene, and ethyl 2-bromo-2-fluoroacetate were involved in Na₂S₂O₄-mediated radical additions to vinyl ethers in the presence of alcohols to give difluoro or monofluoroacetyl-substituted acetals or corresponding difluoromethylphosphonate- and (difluoromethylphenyl)sulfonyl-substituted alkyl acetals. This methodology has also been applied as a key step in the synthesis of hitherto unknown 3,3-difluoro-GABA, completing the series of isomeric difluoro GABAs. Comparison of the pK_a values of 3-fluoro- and 3,3-difluoro-GABA with that of the fluorine free parent compound showed that introduction of each fluorine lead to acidification of both the amino and the carboxyl functions by approximately one unit.

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 LA - eng
 PT - Journal Article
 DEP - 20151125
 PL - United States
 TA - J Org Chem
 JT - The Journal of organic chemistry
 JID - 2985193R
 SB - IM
 EDAT- 2015/11/10 06:00
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 PHST- 2015/11/25 [aheadofprint]
 AID - 10.1021/acs.joc.5b02171 [doi]
 PST - ppublish
 SO - J Org Chem. 2015 Dec 18;80(24):12258-64. doi: 10.1021/acs.joc.5b02171. Epub 2015
 Nov 25.

 PMID- 26626141
 OWN - NLM
 STAT- Publisher
 DA - 20151202
 LR - 20151203
 IS - 1097-458X (Electronic)
 IS - 0749-1581 (Linking)
 DP - 2015 Dec 2
 TI - Monitoring oil displacement processes with k-t accelerated spin echo SPI.
 LID - 10.1002/mrc.4362 [doi]
 AB - Magnetic resonance imaging (MRI) is a robust tool to monitor oil displacement
 processes in porous media. Conventional MRI measurement times can be lengthy,
 which hinders monitoring time-dependent displacements. Knowledge of the oil and
 water microscopic distribution is important because their pore scale behavior
 reflects the oil trapping mechanisms. The oil and water pore scale distribution
 is reflected in the magnetic resonance T2 signal lifetime distribution. In this
 work, a pure phase-encoding MRI technique, spin echo SPI (SE-SPI), was employed
 to monitor oil displacement during water flooding and polymer flooding. A k-t
 acceleration method, with low-rank matrix completion, was employed to improve the
 temporal resolution of the SE-SPI MRI measurements. Comparison to conventional

SE-SPI T2 mapping measurements revealed that the k-t accelerated measurement was more sensitive and provided higher-quality results. It was demonstrated that the k-t acceleration decreased the average measurement time from 66.7 to 20.3 min in this work. A perfluorinated oil, containing no 1 H, and H2 O brine were employed to distinguish oil and water phases in model flooding experiments. High-quality 1D water saturation profiles were acquired from the k-t accelerated SE-SPI measurements. Spatially and temporally resolved T2 distributions were extracted from the profile data. The shift in the 1 H T2 distribution of water in the pore space to longer lifetimes during water flooding and polymer flooding is consistent with increased water content in the pore space. Copyright (c) 2015 John Wiley & Sons, Ltd.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151202

TA - Magn Reson Chem

JT - Magnetic resonance in chemistry : MRC

JID - 9882600

OTO - NOTNLM

OT - 1H

OT - MRI

OT - T2 distribution

OT - enhanced oil recovery

OT - k-t SE-SPI

OT - oil displacement

OT - pore scale fluid behavior

OT - water saturation profile

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PHST- 2015/07/17 [received]
 PHST- 2015/08/31 [revised]
 PHST- 2015/09/03 [accepted]
 AID - 10.1002/mrc.4362 [doi]
 PST - aheadofprint
 SO - Magn Reson Chem. 2015 Dec 2. doi: 10.1002/mrc.4362.

PMID- 26264254
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151215
 IS - 1876-7478 (Electronic)
 IS - 1874-7787 (Linking)
 VI - 24 Pt 3
 DP - 2015 Dec
 TI - Transcriptome of the Antarctic amphipod *Gondogeneia antarctica* and its response to pollutant exposure.
 PG - 253-4
 LID - 10.1016/j.margen.2015.07.012 [doi]
 LID - S1874-7787(15)30004-0 [pii]
 AB - *Gondogeneia antarctica* is widely distributed off the western Antarctic Peninsula and is a key species in the Antarctic food web. In this study, we performed Illumina sequencing to produce a total of 4,599,079,601 (4.6Gb) nucleotides and a comprehensive transcript dataset for *G. antarctica*. Over 46 million total reads were assembled into 20,749 contigs, and 12,461 annotated genes were predicted by Blastx. The RNA-seq results after exposure to three pollutants showed that 658, 169 and 367 genes that were potential biomarkers of responses to pollutants for this species were specifically upregulated after exposure to PCBs (Polychlorinated biphenyls), PFOS (Perfluorooctanesulfonic acid) and PFOA (Perfluorooctanoic acid), respectively. These data represent the first transcriptome resource for the Antarctic amphipod *G. antarctica* and provide a useful resource for studying Antarctic marine species.
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 LA - eng
 PT - Journal Article

DEP - 20150809
 PL - Netherlands
 TA - Mar Genomics
 JT - Marine genomics
 JID - 101475200
 SB - IM
 OTO - NOTNLM
 OT - Amphipod
 OT - Antarctica
 OT - Gondogeneia antarctica
 OT - Transcriptome
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 CRDT- 2015/08/13 06:00
 PHST- 2015/06/28 [received]
 PHST- 2015/07/08 [revised]
 PHST- 2015/07/08 [accepted]
 PHST- 2015/08/09 [aheadofprint]
 AID - S1874-7787(15)30004-0 [pii]
 AID - 10.1016/j.margen.2015.07.012 [doi]
 PST - ppublish
 SO - Mar Genomics. 2015 Dec;24 Pt 3:253-4. doi: 10.1016/j.margen.2015.07.012. Epub 2015 Aug 9.

 PMID- 26506027
 OWN - NLM
 STAT- In-Data-Review
 DA - 20151221
 IS - 1879-3363 (Electronic)
 IS - 0025-326X (Linking)
 VI - 101
 IP - 2
 DP - 2015 Dec 30
 TI - Levels and spatial distribution of perfluoroalkyl substances in China Liaodong Bay basin with concentrated fluorine industry parks.
 PG - 965-71
 LID - 10.1016/j.marpolbul.2015.10.024 [doi]
 LID - S0025-326X(15)30099-0 [pii]
 AB - Eighteen different perfluoroalkyl substances (PFASs) were investigated in 35 river water samples and 34 sediment samples collected from rivers in the Liaodong Bay basin containing two fluorine industry parks. Perfluorooctanoate (PFOA) and perfluorooctane sulfonate (PFOS) were the predominant PFASs in freshwater, with median concentrations of 26.5ng/L and 1.87ng/L, respectively. However, perfluorobutane sulfonate (PFBS) had the highest maximum concentration (up to 124.1ng/L, approximately two orders of magnitude higher) in water at a site which is the nearest to the industrial source of PFASs. Total PFASs in water at this site were also the highest. In contrast, PFOA and perfluorooctadecanoate (PFOcDA) were the most abundant PFASs in sediment, with median concentrations of 1.19ng/g

and 0.35ng/g, respectively. Total PFAS concentrations in sediment from the site near to the industrial park were significantly higher than the other rivers. Mass loading of total PFASs from the rivers flowing into Liaodong Bay was estimated to be 506kg/year.

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LA - eng

PT - Journal Article

DEP - 20151021

PL - England

TA - Mar Pollut Bull

JT - Marine pollution bulletin

JID - 0260231

SB - IM

OTO - NOTNLM

OT - Level

OT - Mass loading

OT - PFASs

OT - Spatial distribution

EDAT- 2015/10/28 06:00

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CRDT- 2015/10/28 06:00

PHST- 2015/08/19 [received]

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PHST- 2015/10/11 [accepted]

PHST- 2015/10/21 [aheadofprint]

AID - S0025-326X(15)30099-0 [pii]

AID - 10.1016/j.marpolbul.2015.10.024 [doi]

PST - ppublish

SO - Mar Pollut Bull. 2015 Dec 30;101(2):965-71. doi: 10.1016/j.marpolbul.2015.10.024.

Epub 2015 Oct 21.

PMID- 26464314

OWN - NLM

STAT- In-Data-Review

DA - 20151120

IS - 1477-0539 (Electronic)

IS - 1477-0520 (Linking)

VI - 13

IP - 46

DP - 2015 Dec 14

TI - Photocatalytic fluoroalkylation reactions of organic compounds.

PG - 11153-83

LID - 10.1039/c5ob01486g [doi]

AB - Photocatalytic methods for fluoroalkyl-radical generation provide more convenient alternatives to the classical perfluoroalkyl-radical (Rf) production through chemical initiators, such as azo or peroxide compounds or the employment of transition metals through a thermal electron transfer (ET) initiation process. The mild photocatalytic reaction conditions tolerate a variety of functional groups and, thus, are handy to the late-stage modification of bioactive molecules. Transition metal-photocatalytic reactions for Rf radical generation profit from the redox properties of coordinatively saturated Ru or Ir organocomplexes to act as both electron donor and reductive species, thus

allowing for the utilization of electron accepting and donating fluoroalkylating agents for Rf radical production. On the other hand, laboratory-available and inexpensive photoorgano catalysts (POC), in the absence of transition metals, can also act as electron exchange species upon excitation, resulting in ET reactions that produce Rf radicals. In this work, a critical account of transition metal and transition metal-free Rf radical production will be described with photoorgano catalysts, studying classical examples and the most recent investigations in the field.

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LA - eng

PT - Journal Article

PT - Review

PL - England

TA - Org Biomol Chem

JT - Organic & biomolecular chemistry

JID - 101154995

SB - IM

EDAT- 2015/10/16 06:00

MHDA- 2015/10/16 06:00

CRDT- 2015/10/15 06:00

AID - 10.1039/c5ob01486g [doi]

PST - ppublish

SO - Org Biomol Chem. 2015 Dec 14;13(46):11153-83. doi: 10.1039/c5ob01486g.

PMID- 26635251

OWN - NLM

STAT- In-Data-Review

DA - 20151218

IS - 1523-7052 (Electronic)

IS - 1523-7052 (Linking)

VI - 17

IP - 24

DP - 2015 Dec 18

TI - Copper-Catalyzed Cyclopropanol Ring Opening Csp(3)-Csp(3) Cross-Couplings with

(Fluoro)Alkyl Halides.

PG - 6074-7

LID - 10.1021/acs.orglett.5b03096 [doi]

AB - Novel and general copper-catalyzed cyclopropanol ring opening cross-coupling reactions with difluoroalkyl bromides, perfluoroalkyl iodides, monofluoroalkyl bromides, and 2-bromo-2-alkylesters to synthesize various beta-(fluoro)alkylated ketones are reported. The reactions feature mild conditions and excellent functional group compatibility and can be scaled up to gram scale. Preliminary mechanistic studies suggest the involvement of radical intermediates. The difluoroalkyl-alkyl cross-coupling products can also be readily converted to more valuable and diverse gem-difluoro-containing compounds by taking advantage of the carbonyl group resulting from cyclopropanol ring opening.

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LA - eng

PT - Journal Article

DEP - 20151204

PL - United States

TA - Org Lett

JT - Organic letters

JID - 100890393

SB - IM

EDAT- 2015/12/05 06:00

MHDA- 2015/12/05 06:00

CRDT- 2015/12/05 06:00

PHST- 2015/12/04 [aheadofprint]

AID - 10.1021/acs.orglett.5b03096 [doi]

PST - ppublish

SO - Org Lett. 2015 Dec 18;17(24):6074-7. doi: 10.1021/acs.orglett.5b03096. Epub 2015 Dec 4.

PMID- 26624992

OWN - NLM

STAT- In-Data-Review

DA - 20151202
 LR - 20151214
 IS - 1932-6203 (Electronic)
 IS - 1932-6203 (Linking)
 VI - 10
 IP - 12
 DP - 2015
 TI - Metabolic Profiling of Chicken Embryos Exposed to Perfluorooctanoic Acid (PFOA) and Agonists to Peroxisome Proliferator-Activated Receptors.
 PG - e0143780
 LID - 10.1371/journal.pone.0143780 [doi]
 AB - Untargeted metabolic profiling of body fluids in experimental animals and humans exposed to chemicals may reveal early signs of toxicity and indicate toxicity pathways. Avian embryos develop separately from their mothers, which gives unique possibilities to study effects of chemicals during embryo development with minimal confounding factors from the mother. In this study we explored blood plasma and allantoic fluid from chicken embryos as matrices for revealing metabolic changes caused by exposure to chemicals during embryonic development. Embryos were exposed via egg injection on day 7 to the environmental pollutant perfluorooctanoic acid (PFOA), and effects on the metabolic profile on day 12 were compared with those caused by GW7647 and rosiglitazone, which are selective agonists to peroxisome-proliferator activated receptor alpha (PPARalpha) and PPARgamma, respectively. Analysis of the metabolite concentrations from allantoic fluid by Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) showed clear separation between the embryos exposed to GW7647, rosiglitazone, and vehicle control, respectively. In blood plasma only GW7647 caused a significant effect on the metabolic profile. PFOA induced embryo mortality and increased relative liver weight at the highest dose. Sublethal doses of PFOA did not significantly affect the metabolic profile in either matrix, although single metabolites appeared to be altered. Neonatal mortality by PFOA in the mouse has been suggested to be mediated via activation of PPARalpha. However, we found no similarity in the metabolite profile of chicken embryos exposed to PFOA with those of embryos exposed to PPAR agonists. This indicates that PFOA does not activate PPAR pathways in our model at concentrations in eggs and embryos well above those found in wild birds. The present study suggests that allantoic fluid and plasma from chicken embryos are useful and complementary matrices for exploring effects on the metabolic profile resulting from chemical exposure during embryonic development.
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LA - eng

PT - Journal Article

DEP - 20151201

PL - United States

TA - PLoS One

JT - PloS one

JID - 101285081

SB - IM

PMC - PMC4666608

OID - NLM: PMC4666608

EDAT- 2015/12/02 06:00

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PHST- 2015 [ecollection]

PHST- 2015/08/17 [received]

PHST- 2015/11/09 [accepted]

PHST- 2015/12/01 [epublish]

AID - 10.1371/journal.pone.0143780 [doi]

AID - PONE-D-15-36164 [pii]

PST - epublish

SO - PLoS One. 2015 Dec 1;10(12):e0143780. doi: 10.1371/journal.pone.0143780. eCollection 2015.

PMID- 26615489

OWN - NLM

STAT- In-Data-Review

DA - 20151222

IS - 1879-1026 (Electronic)

IS - 0048-9697 (Linking)

VI - 543

IP - Pt A

DP - 2016 Feb 1

TI - Bioaccumulation of perfluorinated carboxylates and sulfonates and polychlorinated biphenyls in laboratory-cultured *Hexagenia* spp., *Lumbriculus variegatus* and *Pimephales promelas* from field-collected sediments.

PG - 715-26

LID - 10.1016/j.scitotenv.2015.11.062 [doi]

LID - S0048-9697(15)31043-3 [pii]

AB - Polychlorinated biphenyls (PCBs) and perfluorinated carboxylates and sulfonates (PFASs) are persistent pollutants in sediment that can potentially bioaccumulate in aquatic organisms. The current study investigates variation in the accumulation of PCBs and PFASs in laboratory-cultured *Hexagenia* spp., *Lumbriculus*

variegatus and Pimephales promelas from contaminated field-collected sediment using 28-day tests. BSAF(lipid) (lipid-normalized biota-sediment accumulation factor) values for total concentration of PCBs were greater in Hexagenia spp. relative to L. variegatus and P. promelas. The distribution of congeners contributing to the total concentration of PCBs in tissue varied among the three species. Trichlorobiphenyl congeners composed the greatest proportion of the total concentration of PCBs in L. variegatus while tetra- and pentabiphenyl congeners dominated in Hexagenia spp. and P. promelas. Perfluorooctane sulfonate (PFOS) was present in all three species at concentrations greater than all other PFASs analyzed. Hexagenia spp. also produced the greatest BSAF(lipid) and BSAF(ww) (non-lipid-normalized biota-sediment accumulation factor) values for PFOS relative to the other two species. However, this was not the case for all PFASs. The trend of BSAF values and number of carbon atoms in the perfluoroalkyl chain of perfluorinated carboxylates varied among the three species but was similar for perfluorinated sulfonates. Differences in the dominant pathways of exposure (e.g., water, sediment ingestion) likely explain a large proportion of the variation in accumulation observed across the three species.

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LA - eng

PT - Journal Article

DEP - 20151207

PL - Netherlands

TA - Sci Total Environ

JT - The Science of the total environment

JID - 0330500

SB - IM

OTO - NOTNLM

OT - Aquatic invertebrates

OT - Bioaccumulation

OT - PFASs
 OT - PFOS
 OT - Polychlorinated biphenyls
 OT - Sediment
 EDAT- 2015/11/30 06:00
 MHDA- 2015/11/30 06:00
 CRDT- 2015/11/30 06:00
 PHST- 2015/09/15 [received]
 PHST- 2015/11/12 [revised]
 PHST- 2015/11/12 [accepted]
 PHST- 2015/12/07 [aheadofprint]
 AID - S0048-9697(15)31043-3 [pii]
 AID - 10.1016/j.scitotenv.2015.11.062 [doi]
 PST - ppublish
 SO - Sci Total Environ. 2016 Feb 1;543(Pt A):715-26. doi:
 10.1016/j.scitotenv.2015.11.062. Epub 2015 Dec 7.

 PMID- 26674688
 OWN - NLM
 STAT- Publisher
 DA - 20151217
 LR - 20151218
 IS - 1879-1026 (Electronic)
 IS - 0048-9697 (Linking)
 VI - 544
 DP - 2015 Dec 9
 TI - Perfluorinated carboxylic acids in human breast milk from Spain and estimation of
 infant's daily intake.
 PG - 595-600
 LID - S0048-9697(15)31040-8 [pii]
 LID - 10.1016/j.scitotenv.2015.11.059 [doi]
 AB - Human milk samples were collected from 67 mothers in 2014 at a Primary Care
 Centre in Murcia (Spain) and analyzed for perfluorinated carboxylic acids
 (PFCAs). Concentrations measured for perfluorooctanoic acid (PFOA),
 perfluorononanoic acid (PFNA), perfluorodecanoic acid (PFDA), perfluoroundecanoic
 acid (PFUnDA) and perfluorododecanoic acid (PFDoDA) ranged from <LOQ (<10ng/L) to
 397ng/L with a mean concentration of 66+/-68ng/L and a median of 29ng/L. The
 presence of these compounds was revealed in 50 samples out of 67 analyzed.
 Influence of number of pregnancies and food habits on PFCAs concentrations was
 also investigated. Statistically significant differences in PFCA levels were
 found when the women were divided into maternal age classes and into the
 categories primiparae and multiparae. A greater transfer of PFC during
 breastfeeding by primiparous was evidenced and thus a higher exposure to these
 contaminants for the first child. Moreover, it was possible to hypothesize that
 the content of PFCs is in general correlated to the eating habits of donors and,
 in particular, with the fish consumption. Finally, PFOA daily intakes and risk
 index (RI) were estimated for the first six months of life and we found that
 ingestion rates of PFOA did not exceed the tolerable daily intake (TDI)

recommended by the European Food Safety Authority (EFSA).

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151209

TA - Sci Total Environ

JT - The Science of the total environment

JID - 0330500

OTO - NOTNLM

OT - Daily intake

OT - GC-MS

OT - Human milk

OT - PFCAs

OT - PFOA
 OT - Spain
 EDAT- 2015/12/18 06:00
 MHDA- 2015/12/18 06:00
 CRDT- 2015/12/18 06:00
 PHST- 2015/09/26 [received]
 PHST- 2015/11/11 [revised]
 PHST- 2015/11/11 [accepted]
 AID - S0048-9697(15)31040-8 [pii]
 AID - 10.1016/j.scitotenv.2015.11.059 [doi]
 PST - aheadofprint
 SO - Sci Total Environ. 2015 Dec 9;544:595-600. doi: 10.1016/j.scitotenv.2015.11.059.

PMID- 26327633
 OWN - NLM
 STAT- In-Process
 DA - 20151010
 IS - 1879-1026 (Electronic)
 IS - 0048-9697 (Linking)
 VI - 538
 DP - 2015 Dec 15
 TI - Evaluating the impact of a fluoropolymer plant on a river macrobenthic community by a combined chemical, ecological and genetic approach.
 PG - 654-63
 LID - 10.1016/j.scitotenv.2015.08.086 [doi]
 LID - S0048-9697(15)30589-1 [pii]

AB - Effect-based monitoring is a recommended approach suggested in European Guidelines to assess the response of ecosystem affected by a pollution source, considering the effects at community, population, individual but also at suborganism level. A combined chemical, ecological and genetic approach was applied in order to assess the impact of a fluoropolymer plant on the macrobenthic community of the Northern Italian river Bormida (Piedmont region). The macrobenthic community living downstream of the industrial discharge was chronically exposed to a mixture of perfluoroalkyl substances (PFAS), with perfluorooctanoic acid as the main compound, at concentrations up to several $\mu\text{g L}^{-1}$. Ecological assessment proved that the downstream community was not substantially different from that living upstream of the pollution source. The impact on community is not quantifiable with the traditional monitoring methods used for ecological classification under European regulation because macrobenthic communities showed only slight differences in their structure. In order to highlight effects on genetic variability of the native population, a subcellular analysis by using the AFLP (Amplified Fragment Length Polymorphism) genetic technique was applied to genotype of individuals of a selected species (*Hydropsyche modesta*, Trichoptera) collected in the two sampling sites. Percentage of variation between the two populations was 6.8%, a threshold compatible with a genetic drift induced in the downstream population. The genetic study carried out in field identified a significant divergence between exposed and non-exposed populations, but at present it is not possible to associate this

divergence to a specific effect induced by PFAS.

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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

DEP - 20150829

PL - Netherlands

TA - Sci Total Environ

JT - The Science of the total environment

JID - 0330500

SB - IM

OTO - NOTNLM

OT - Benthic invertebrates

OT - Effect-based monitoring

OT - Genetic selection

OT - PFOA

EDAT- 2015/09/04 06:00
 MHDA- 2015/09/04 06:00
 CRDT- 2015/09/02 06:00
 PHST- 2015/05/20 [received]
 PHST- 2015/08/14 [revised]
 PHST- 2015/08/15 [accepted]
 PHST- 2015/08/29 [aheadofprint]
 AID - S0048-9697(15)30589-1 [pii]
 AID - 10.1016/j.scitotenv.2015.08.086 [doi]
 PST - ppublish
 SO - Sci Total Environ. 2015 Dec 15;538:654-63. doi: 10.1016/j.scitotenv.2015.08.086.
 Epub 2015 Aug 29.

PMID- 26318684
 OWN - NLM
 STAT- In-Process
 DA - 20151010
 IS - 1879-1026 (Electronic)
 IS - 0048-9697 (Linking)
 VI - 538
 DP - 2015 Dec 15
 TI - Perfluorinated sulfonate and carboxylate compounds and precursors in herring gull eggs from across the Laurentian Great Lakes of North America: Temporal and recent spatial comparisons and exposure implications.
 PG - 468-77
 LID - 10.1016/j.scitotenv.2015.08.083 [doi]
 LID - S0048-9697(15)30586-6 [pii]
 AB - Chemicals of emerging concern (CECs) in the basin of the Laurentian Great Lakes of North America include per- and poly-fluoroalkyl substances (PFASs) classified as perfluoroalkyl acids. We investigated several PFASs, and specifically 13 C4-C16 perfluorinated carboxylic acids (PFCAs), 4 (C4, C6, C8 and C10) perfluorinated sulfonates (PFSA), perfluoro-4-ethylcyclohexane sulfonate (PFEtCHxS) and selected precursors (e.g. perfluorobutane sulfonamide and perfluorooctane sulfonamide) in herring gull (*Larus argentatus*) eggs collected in 2012-2013 from 19 Canadian and U.S. colony sites across the Great Lakes. C6, C8 and C10 PFSA, PFEtCHxS, and C7-14 and C16 PFCAs were quantifiable at >97% of the 114 egg samples. PFEtCHxS concentrations ranged from n.d. to 3.1ng/g ww (highest in Lake Michigan eggs). Mean Sigma4PFSA (92 to 97% perfluorooctane sulfonate (PFOS)) and Sigma9PFCA concentration ranges were 44 to 740 and 4.8 to 118ng/g ww, respectively. Sigma4PFSA showed a clear increasing concentration trend from the northwest to the southeast colonies. Also, Sigma4PFCA to Sigma9PFSA concentration ratios in gull eggs were greater in eggs from Lake Superior relative to colonies in the other lakes. PFOS concentrations in some egg samples were greater than some of the known lowest observed effect concentrations (LOECs) measured and reported in captive bird model studies. This study showed the increasing complexity of PFAS-CECs, and emphasized the importance of continuing monitoring of bioaccumulative PFAS in Great Lakes herring gulls.
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LA - eng
PT - Journal Article
PT - Research Support, Non-U.S. Gov't
PT - Research Support, U.S. Gov't, Non-P.H.S.
DEP - 20150827
PL - Netherlands
TA - Sci Total Environ
JT - The Science of the total environment
JID - 0330500
SB - IM
OTO - NOTNLM
OT - Eggs
OT - Herring gull
OT - Laurentian Great Lakes
OT - PFOS
OT - Perfluorinated carboxylic acids
OT - Perfluorinated sulfonates
EDAT- 2015/09/01 06:00

MHDA- 2015/09/01 06:00
 CRDT- 2015/08/31 06:00
 PHST- 2015/07/21 [received]
 PHST- 2015/08/14 [revised]
 PHST- 2015/08/15 [accepted]
 PHST- 2015/08/27 [aheadofprint]
 AID - S0048-9697(15)30586-6 [pii]
 AID - 10.1016/j.scitotenv.2015.08.083 [doi]
 PST - ppublish
 SO - Sci Total Environ. 2015 Dec 15;538:468-77. doi: 10.1016/j.scitotenv.2015.08.083.
 Epub 2015 Aug 27.

PMID- 26666359
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160107
 IS - 1878-5867 (Electronic)
 IS - 0039-128X (Linking)
 VI - 105
 DP - 2016 Jan
 TI - Estrone sulfate and dehydroepiandrosterone sulfate: Transactivation of the
 estrogen and androgen receptor.
 PG - 50-8
 LID - 10.1016/j.steroids.2015.11.009 [doi]
 LID - S0039-128X(15)00296-2 [pii]
 AB - Dehydroepiandrosterone sulfate (DHEAS) and estrone sulfate (E1S) are two of the
 most abundant steroids in the human circulation. The enzyme steroid sulfatase
 (STS) cleaves the sulfate group of DHEAS and E1S leading to biosynthesis of
 endogenous hormones such as testosterone and estrone. In the current study we
 aimed at determining the effect of E1S and DHEAS on estrogen receptor (ER) and
 androgen receptor (AR) transactivation. Using luciferase reporter gene assays,
 the ER and AR transactivities of E1S and DHEAS were determined by direct cell
 exposure; as well as upon extraction from human serum using a method to extract
 perfluorinated alkyl acids (PFAAs). By direct cell exposure, both E1S and DHEAS
 transactivated the ER and the AR in dose-dependent manners. The DHEAS-induced AR
 transactivity could be abolished by the STS inhibitor STX64. Immunoassay analysis
 confirmed the presence of E1S and DHEAS in the serum PFAA extracts with mean
 recoveries below 2.5%. For the PFAA extracts of human male and female serum, only
 the AR was significantly transactivated. The AR transactivity of the sulfated
 steroids in the extracts was abolished by STX64 to obtain the net PFAA induced
 xenohormone transactivity, but further cleanup might be needed at high
 concentrations of E1S.

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LA - eng
PT - Journal Article
DEP - 20151205
PL - United States
TA - Steroids
JT - Steroids
JID - 0404536
SB - IM
OTO - NOTNLM
OT - Androgen receptor
OT - Dehydroepiandrosterone sulfate
OT - Estrogen receptor
OT - Estrone sulfate
OT - Perfluorinated compounds
OT - Steroid sulfatase
EDAT- 2015/12/17 06:00
MHDA- 2015/12/17 06:00
CRDT- 2015/12/16 06:00
PHST- 2015/07/03 [received]
PHST- 2015/10/15 [revised]
PHST- 2015/11/27 [accepted]
PHST- 2015/12/05 [aheadofprint]
AID - S0039-128X(15)00296-2 [pii]
AID - 10.1016/j.steroids.2015.11.009 [doi]
PST - ppublish
SO - Steroids. 2016 Jan;105:50-8. doi: 10.1016/j.steroids.2015.11.009. Epub 2015 Dec 5.

PMID- 26459446

OWN - NLM

STAT- In-Process

DA - 20151013

IS - 1873-3573 (Electronic)

IS - 0039-9140 (Linking)

VI - 145

DP - 2015 Dec 1

TI - Reprint of 'Draw your assay: Fabrication of low-cost paper-based diagnostic and multi-well test zones by drawing on a paper'.

PG - 73-7

LID - 10.1016/j.talanta.2015.09.042 [doi]

LID - S0039-9140(15)00434-8 [pii]

AB - Interest in low-cost diagnostic devices has recently gained attention, in part due to the rising cost of healthcare and the need to serve populations in resource-limited settings. A major challenge in the development of such devices is the need for hydrophobic barriers to contain polar bio-fluid analytes. Key approaches in lowering the cost in diagnostics have centered on (i) development of low-cost fabrication techniques/processes, (ii) use of affordable materials, or, (iii) minimizing the need for high-tech tools. This communication describes a simple, low-cost, adaptable, and portable method for patterning paper and subsequent use of the patterned paper in diagnostic tests. Our approach generates hydrophobic regions using a ball-point pen filled with a hydrophobizing molecule suspended in a solvent carrier. An empty ball-point pen was filled with a solution of trichloro perfluoroalkyl silane in hexanes (or hexadecane), and the pen used to draw lines on Whatman(R) chromatography 1 paper. The drawn regions defined the test zones since the trichloro silane reacts with the paper to give a hydrophobic barrier. The formation of the hydrophobic barriers is reaction kinetic and diffusion-limited, ensuring well defined narrow barriers. We performed colorimetric glucose assays and enzyme-linked immuno-sorbent assay (ELISA) using the created test zones. To demonstrate the versatility of this approach, we fabricated multiple devices on a single piece of paper and demonstrated the reproducibility of assays on these devices. The overall cost of devices fabricated by drawing are relatively lower (<US \$0.001 per device) than those derived from wax-printing (US\$0.05-0.003) or other approaches.

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LA - eng
PT - Journal Article
PL - Netherlands
TA - Talanta
JT - Talanta
JID - 2984816R
RPF - Talanta. 2015 Nov 1;144:289-93. PMID: 26452824
OTO - NOTNLM
OT - Low-cost devices
OT - Paper-based devices
OT - Point of care diagnostics
OT - p-ELISA
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STAT- In-Data-Review
DA - 20151126
LR - 20151215
IS - 1096-0333 (Electronic)
IS - 0041-008X (Linking)
VI - 289
IP - 3
DP - 2015 Dec 15
TI - Application of physiologically-based pharmacokinetic modeling to explore the role of kidney transporters in renal reabsorption of perfluorooctanoic acid in the rat.
PG - 428-41
LID - 10.1016/j.taap.2015.10.017 [doi]
LID - S0041-008X(15)30120-4 [pii]
AB - Renal elimination and the resulting clearance of perfluorooctanoic acid (PFOA) from the serum exhibit pronounced sex differences in the adult rat. The literature suggests that this is largely due to hormonally regulated expression of organic anion transporters (OATs) on the apical and basolateral membranes of the proximal tubule cells that facilitate excretion and reabsorption of PFOA from the filtrate into the blood. Previously developed PBPK models of PFOA exposure in the rat have not been parameterized to specifically account for transporter-mediated renal elimination. We developed a PBPK model for PFOA in male and female rats to explore the role of Oat1, Oat3, and Oatplal in sex-specific renal reabsorption and excretion of PFOA. Descriptions of the kinetic behavior of these transporters were extrapolated from in vitro studies and the model was used to simulate time-course serum, liver, and urine data for intravenous (IV) and oral exposures in both sexes. Model predicted concentrations of PFOA in the liver, serum, and urine showed good agreement with experimental data for both male and female rats indicating that in vitro derived physiological descriptions of transporter-mediated renal reabsorption can successfully predict sex-dependent excretion of PFOA in the rat. This study supports the hypothesis that sex-specific serum half-lives for PFOA are largely driven by expression of transporters in the kidney and contribute to the development of PBPK modeling as a tool for evaluating the role of transporters in renal clearance.
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 PT - Journal Article
 DEP - 20151106
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 TA - Toxicol Appl Pharmacol
 JT - Toxicology and applied pharmacology
 JID - 0416575
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 PMC - PMC4662604
 MID - HHSPA738119
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 OTO - NOTNLM
 OT - IVIVE
 OT - Oat1
 OT - Oat3
 OT - Oatpla1
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 VI - 148
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 TI - Chronic Exposure of Female Mice to an Environmental Level of Perfluorooctane

Sulfonate Suppresses Estrogen Synthesis Through Reduced Histone H3K14 Acetylation of the StAR Promoter Leading to Deficits in Follicular Development and Ovulation.

PG - 368-79

LID - 10.1093/toxsci/kfv197 [doi]

AB - Perfluorooctane sulfonate (PFOS) at a high dose of 10 mg/kg has been reported to affect the neuroendocrine system and exert toxic effects in rodents. The present study examined the influence of chronic exposure to a low-dose of PFOS (0.1 mg/kg/day) on female reproductive endocrine and function. Herein, we show that adult female mice exposed to PFOS by gavage for 4 months (PFOS-mice) exhibited a prolongation of diestrus without signs of toxic effects. The numbers of mature follicles and corpora luteum were significantly reduced in PFOS-mice with increase of atresic follicles. The levels of serum estrogen (E2) and progesterone at proestrus and diestrus were reduced in PFOS-mice. In comparison with controls, PFOS-mice showed a significant decrease in the levels of luteinizing hormone (LH) and follicle stimulating hormone (FSH), and gonadotrophin-releasing hormone, the number of kisspeptin neurons and the level of kiss1 mRNA in anteroventral periventricular nucleus at proestrus but not at diestrus, which could be corrected with the normalization to E2. PFOS-mice did not generate an LH-surge at proestrus, which could be rescued by the application of E2 or kisspeptin-10. Notably, the level of ovarian steroidogenic acute regulatory (StAR) mRNA was decreased in PFOS-mice with the reduction of histone H3K14 acetylation in StAR promoter relative to control mice, whereas the P450scc expression and histone H3K14 acetylation showed no difference between the groups. The present study provides evidence that the chronic exposure to the low-dose of PFOS through selectively reducing histone acetylation of StAR suppresses the biosynthesis of E2 to impair the follicular development and ovulation.

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PL - United States

TA - Toxicol Sci

JT - Toxicological sciences : an official journal of the Society of Toxicology

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SB - IM

OTO - NOTNLM

OT - estrogen (E2)

OT - histone acetylation

OT - hypothalamic-pituitary-gonadal (HPG) axis

OT - perfluorooctane sulfonate (PFOS)

OT - steroidogenic acute regulatory (StAR)

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AID - kfv197 [pii]

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VI - 91

DP - 2015 Dec 30

TI - Use of strong anion exchange resins for the removal of perfluoroalkylated
substances from contaminated drinking water in batch and continuous pilot plants.

PG - 137-146

LID - S0043-1354(15)30437-1 [pii]

LID - 10.1016/j.watres.2015.12.039 [doi]

AB - In recent years abnormally high levels of perfluoroalkylated substances (PFAS)
have been detected both in surface and underground water sampled in an area
covering approximately 150 square kilometers in the Veneto region (Italy)
indicating the presence of a pollution point source (fluorochemicals production
plant). Adsorption on granular activated carbon is an emergency measure which is
poorly effective requiring frequent replacement. This work focuses on the
application of three strong anion exchange resins (Purolite(R) A520E, A600E and
A532E) for the removal of traces of PFOA, PFOS, PFBA and PFBS (concentration of
hundreds of ng L⁻¹) from drinking water. This technology is attractive for the

possibility of reusing resins after an in-situ regeneration step. A strong relationship between the hydrophobicity of the exchange functional group of the resin and its capacity in removing PFAS exists. A600E (non hydrophobic) and A520E (fairly hydrophobic) show a reduced sorption capacity compared to A532E (highly hydrophobic). While A600E and A520E can be regenerated with solvent-less dilute solutions of non-toxic NH₄Cl and NH₄OH, A532E requires concentrated solutions of methanol or ethanol and 1% NH₄Cl and for the sake of this work it was regarded as non-regenerable. The volume of regeneration effluents requiring incineration can be efficiently reduced by more than 96.5% by using reverse osmosis coupled with under-vacuum evaporation. Transmission electron analysis on saturated resins showed that large molecular macro-aggregates of PFAS can form in the intraparticle pores of resin indicating that ion exchange is not the only mechanism involved in PFAS removal.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20151230

TA - Water Res

JT - Water research

JID - 0105072

OTO - NOTNLM

OT - Anion exchange resin

OT - Granular activated carbon

OT - Ion exchange

OT - PFAS

OT - Removal

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 DA - 20151209
 LR - 20151210
 IS - 1097-0061 (Electronic)
 IS - 0749-503X (Linking)
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 TI - Cloning and evaluation of different constitutive promoters in the oleaginous yeast *Rhodospiridium toruloides*.
 LID - 10.1002/yea.3145 [doi]
 AB - The oleaginous yeast *Rhodospiridium toruloides* is an unconventional yeast species that can accumulate a high content of lipids. Because it belongs to basidiomycetous fungus, limited tools and functional elements are available for genetic engineering of *R. toruloides* and related red yeasts. Here we report the functional evaluation of five constitutive promoters from this yeast. We assembled reporter gene expression cassette consisted of a promoter, the hygromycin gene (HYG) and the nos terminator, and inserted into the binary vector pZPK. Hygromycin resistant transformants were obtained when *R. toruloides* cells were co-cultured with *Agrobacterium tumefaciens* AGL1 cells harboring the engineered vector. Genomic integration of the reporter cassette was verified by successful amplification of target DNA fragments. Quantitative PCR analysis suggested that the transformant had only one copy of the reporter cassette. The strength of these promoters was demonstrated at the phenotypic level on the hygromycin-gradient plate and at the transcriptional level by real-time quantitative PCR. It was found that the strengths of these promoters varied no more than fivefold and followed a decreasing sequence of PPGI, PPGK, PFBA, PTPI, and PGPD. This study established new genetic elements for the construction of superior *R. toruloides* strains to produce advanced biofuels and related chemicals.
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TA - Yeast
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